High-recall causal discovery for autocorrelated time series with latent confounders

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Abstract

We present a new method for linear and nonlinear, lagged and contemporaneous constraint-based causal discovery from observational time series in the presence of latent confounders. We show that existing causal discovery methods such as FCI and variants suffer from low recall in the autocorrelated time series case and identify low effect size of conditional independence tests as the main reason. Information-theoretical arguments show that effect size can often be increased if causal parents are included in the conditioning sets. To identify parents early on, we suggest an iterative procedure that utilizes novel orientation rules to determine ancestral relationships already during the edge removal phase. We prove that the method is order-independent, and sound and complete in the oracle case. Extensive simulation studies for different numbers of variables, time lags, sample sizes, and further cases demonstrate that our method indeed achieves much higher recall than existing methods while keeping false positives at the desired level. This performance gain grows with stronger autocorrelation. Our method also covers causal discovery for non-time series data as a special case. We provide Python code for all methods involved in the simulation studies.

1 Introduction

Observational causal discovery [Spirtes et al., 2000, Peters et al., 2017] from time series is a challenge of high relevance to many fields of science and engineering if experimental interventions are infeasible, expensive, or unethical. Causal knowledge of direct and indirect effects, interaction pathways, and time lags can help to understand and model physical systems and to predict the effect of interventions [Pearl, 2000]. Causal graphs can also guide interpretable variable selection for prediction and classification tasks. Causal discovery from time series faces major challenges [Runge et al., 2019a] such as unobserved confounders, high-dimensionality, and nonlinear dependencies, to name a few. Few frameworks can deal with these challenges and we here focus on constraint-based methods pioneered in the seminal works of Spirtes, Glymour, and Zhang [Spirtes et al., 2000, Zhang, 2008]. We demonstrate that existing latent causal discovery methods strongly suffer from low recall in the time series case where identifying lagged and contemporaneous causal links is the goal and autocorrelation is an added, ubiquitous challenge. Our main theoretical contributions lie in identifying low effect size as a major reason why current methods fail and introducing a novel sound, complete, and order-independent causal discovery algorithm that yields strong gains in recall. Our practical contributions lie in extensive numerical experiments that can serve as a future benchmark and open-source Python implementations of our and major previous time series causal discovery algorithms. The paper is structured as follows: After briefly introducing the problem and existing methods in Sec. 2, we describe our method and theoretical results in Sec. 3.
Section 4 provides numerical experiments followed by a discussion of strengths and weaknesses and an outlook in Sec. 5. The paper is accompanied by Supplementary Material (SM).

2 Time series causal discovery in the presence of latent confounders

2.1 Preliminaries

We consider multivariate time series \( V^j = (V^j_t, V^j_{t-1}, \ldots) \) for \( j = 1, \ldots, \tilde{N} \) that follow a stationary discrete-time structural vector-autoregressive process described by the structural causal model (SCM)

\[
V^j_i = f_j(p_a(V^j_i), \eta^j_i) \quad \text{with} \quad j = 1, \ldots, \tilde{N}.
\]

The measurable functions \( f_j \) depend non-trivially on all their arguments, the noise variables \( \eta^j_i \) are jointly independent, and the sets \( p_a(V^j_i) \subseteq (V^j_t, V^j_{t-1}, \ldots, V^j_{t-p^j}) \) define the causal parents of \( V^j_i \). Here \( V_t = (V^1_t, V^2_t, \ldots) \) and \( p^j \) is the order of the time series. Due to stationarity the causal relationship of the pair of variables \( (V^j_{t-\tau}, V^j_t) \) is the same as that of all time shifted pairs \( (V^j_{1-\tau}, V^j_1) \). This is why below we always fix one variable at time \( t \) and take \( \tau \geq 0 \). We assume that there are no cyclic causal relationships, which as a result of time order restricts the contemporaneous (\( \tau = 0 \)) interactions only. We allow for unobserved variables, i.e., we allow for observing only a subset \( X = \{X^1, \ldots, X^N\} \subseteq V = \{V^1, V^2, \ldots\} \) of time series with \( N \leq \tilde{N} \). We further assume that there are no selection variables and assume the faithfulness [Spirtes et al., 2000] condition, which states that conditional independence (CI) in the observed distribution \( P(V) \) generated by the SCM implies d-separation in the associated time series graph \( G \) over variables \( V \).

We assume the reader is familiar with the Fast Causal Inference (FCI) algorithm [Spirtes et al., 1995, 2000, Zhang, 2008] and related graphical terminology, see secs. S1 and S2 of the SM for a brief overview. Importantly, the relevant MAGs (maximal ancestral graphs) can contain directed (\( \rightarrow \)) and bidirected (\( \leftrightarrow \)) edges (links). In the associated PAGs (partial ancestral graphs) there additionally may be edges of the type (\( \rightarrow \rightarrow \)) and (\( \leftrightarrow \leftrightarrow \)).

2.2 Existing methods

The tsFCI algorithm [Entner and Hoyer, 2010] adapts the constraint-based FCI algorithm to time series. It uses time order and stationarity to restrict conditioning sets and to apply additional edge orientations. SVAR-FCI [Malinsky and Spirtes, 2018] uses stationarity to also infer additional edge removals. There are no assumptions on the functional relationships or on the structure of confounding. Granger causality [Granger, 1969] is another common framework for inferring the causal structure of time series. It cannot deal with contemporaneous links (known as instantaneous effects in this context) and may draw wrong conclusions in the presence of latent confounders, see e.g. [Peters et al., 2017] for an overview. The ANLTSAM method [Chu and Glymour, 2008] restricts contemporaneous interactions to be linear, and latent confounders to be linear and contemporaneous. TS-LiNGAM [Hyvärinen et al., 2008] is based on LiNGAM [Shimizu et al., 2006] rooted in the structural causal model framework [Peters et al., 2017, Zhang and Spirtes, 2016]. It allows for contemporaneous effects, assumes linear interactions with additive non-Gaussian noise, and might fail in the presence of confounding. The TiMINo [Peters et al., 2013] method restricts interactions to an identifiable function class or requires an acyclic summary graph. Yet another approach are Bayesian score-based or hybrid methods [ Chickering, 2002, Tsamardinos et al., 2006]. These often become computationally infeasible in the presence of unobserved variables, see [Jabbari et al., 2017] for a discussion, or make restrictive assumptions about functional dependencies or variable types.

In this paper we follow the constraint-based approach that allows for general functional relationships (both for lagged and contemporaneous interactions), general types of variables (discrete and continuous, univariate and multivariate), and that makes no assumption on the structure of confounding. The price of this generality is that we will not be able to distinguish members of a Markov equivalence class. Due to its additional use of stationarity, we choose SVAR-FCI rather than tsFCI as a baseline and implement the method, restricted to no selection variables, in Python. As a second baseline we implement a time series adaption of RFCI (also restricted to no selection variables). The RFCI algorithm [Colombo et al., 2012] is a modification of FCI that does not execute the potentially time consuming second edge removal phase based on Possible-D-Sep sets.
2.3 On maximum time lag, stationarity, soundness, and completeness

In time series causal discovery, the assumption of stationarity and the length of the chosen time lag window \( t - \tau_{\text{max}} \leq t' \leq t \) play an important role. In the causally sufficient case \( (X = V) \), the causual graph stays the same for all \( \tau_{\text{max}} \geq p_{ts} \). This is different in the latent case: Let \( \mathcal{M}(\mathcal{G})^{\tau_{\text{max}}} \) be the MAG obtained by marginalizing over all unobserved variables and also all generally observed variables at times \( t' < t - \tau_{\text{max}} \). Then increasing \( \tau_{\text{max}} \) may change also those edges that are fully contained in the original time lag window (both orientations and adjacencies), even in the case of perfect statistical decisions. Hence, \( \tau_{\text{max}} \) may be regarded more as an analysis choice than as a tunable parameter. Second, stationarity also affects the definition of MAGs and PAGs. For example, SVAR-FCI uses stationarity to also remove edges whose separating set extends beyond the chosen time lag window and, hence, does in general not determine a PAG of \( \mathcal{M}(\mathcal{G})^{\tau_{\text{max}}} \). To formalize this let \( i) \mathcal{M}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \) be the MAG obtained from \( \mathcal{M}(\mathcal{G})^{\tau_{\text{max}}} \) by enforcing repeating adjacencies, let \( ii) \mathcal{P}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \) be the maximally informative PAG for the Markov equivalence class of \( \mathcal{M}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \) (from running the FCI orientation rules on \( \mathcal{M}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \)), and let \( iii) \mathcal{P}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \) be the PAG obtained when additionally enforcing time order and repeating orientations at each step. Note that \( \mathcal{P}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \) may have fewer circle marks, i.e., may be more informative than \( \mathcal{P}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \). Our aim is to estimate \( \mathcal{P}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \). We say an algorithm is sound if it returns a PAG for \( \mathcal{M}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \), and complete if it returns \( \mathcal{P}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \).

Below we write \( \mathcal{M}(\mathcal{G}) = \mathcal{M}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \) and \( \mathcal{P}(\mathcal{G}) = \mathcal{P}(\mathcal{G})^{\tau_{\text{max}}}_{\text{statAO}} \) for simplicity. When speaking of FCI and RFCI from here this refers to SVAR-FCI and our time series version of RFCI.

2.4 Motivational example

We illustrate the challenge posed by unobserved variables with the example of Fig. 1. FCI with the partial correlation (ParCorr) CI test correctly identifies the auto-links but misses the true lagged link \( Y_{t-1} \rightarrow Z_t \) and returns a false link \( Y_{t-2} \rightarrow Z_t \) instead. In most realizations FCI fails to detect the contemporaneous adjacency \( X_t \leftrightarrow Y_t \) and, if detected, fails to orient it as bidirected. The reason are wrong CI tests in the edge removal and orientation phases of FCI. When FCI iterates through conditioning sets of cardinality \( p = 0 \) in the edge removal phase, the correlation \( \rho(X_t; Y_t) \) can be non-significant in many realizations since the high autocorrelation of both \( X \) and \( Y \) increases their variance and decreases their signal-to-noise ratio (the common signal due to the latent confounder). Further, for \( p = 1 \) also the lagged correlation \( \rho(Y_{t-1}; Z_t|Y_{t-2}) \) often becomes non-significant and the true link \( Y_{t-1} \rightarrow Z_t \) gets removed. Here conditioning away the autocorrelation of \( Y_{t-1} \) decreases the signal while the noise level in \( Z_t \) is still high due to \( Z \)'s autocorrelation. This false negative has implications for further CI tests since \( Y_{t-1} \) won’t be used in subsequent conditioning sets: the path \( Y_{t-2} \rightarrow Y_{t-1} \rightarrow Z_t \) can then not be blocked anymore and the false positive \( Y_{t-2} \rightarrow Z_t \) remains even after the next removal phase. In the FCI orientation phase rule \( R1 \) yields tails for all auto-links. Even if the link \( X_t \rightarrow Y_t \) is detected, it is in most cases not oriented correctly. The reason again lies in wrong CI tests: In principle the collider rule \( R0 \) should identify \( X_t \leftrightarrow Y_t \) since the middle node of the triple \( X_{t-1} \rightarrow Y_{t-1} \rightarrow Y_t \) does not lie in the separating set of \( X_{t-1} \) and \( Y_t \) (and similarly for \( X \) and \( Y \) swapped). In practice \( R0 \) is implemented with the majority rule [Colombo and Maathuis, 2014] to avoid order-dependence, which involves further CI test given subsets of the adjacencies of \( X_{t-1} \) and

![Figure 1: Latent confounder example of the model in eq. (3) (Sec. 4) with linear ground truth links shown for the LPCMCI case (right panel). All auto-coefficients are 0.9, all cross-coefficients are 0.6 (colored links), false links or links with false orientations are grey. True and false adjacency detection rates shown as link width. Detection rates based on 500 realizations run at \( \alpha = 0.01 \) for \( T = 500 \).](image-url)
We state the theorem in an information theoretic framework with \(I\). Autocorrelation is only one manifestation of a more general problem we observe here: Low signal-to-noise ratio due to an ‘unfortunate’ choice of conditioning sets that leads to low effect size (here partial correlation) and, hence, low statistical power of CI tests. Wrong CI tests then lead to missing links, and these in turn to false positives and wrong orientations. In the following we analyze effect size more theoretically and suggest a general idea to overcome this issue.

3 Latent PCMCI

3.1 Effect size in causal discovery

FCI performs many CI tests, both for removing wrong adjacencies and in majority-based orientation rules. The detection power of true links \(X_{i \rightarrow r} \rightarrow X_{j}^r\) depends on \(i\) sample size (usually fixed), \(ii\) the significance level \(\alpha\) (fixed by the researcher as the desired false positives level), \(iii\) the CI tests’ estimation dimensions (kept at a minimum by FCI’s design to preferentially test small conditioning sets), and \(iv\) the effect size. We here define effect size as the minimum CI test statistic value \(\min_{\hat{\theta}} I(X_{i \rightarrow r}; X_j^r | \hat{S})\) over all conditioning sets \(\hat{S}\) tested by FCI (these are at least all subsets of the adjacencies of \(X_{i \rightarrow r}\) and \(X_{j}^r\), assuming that no true links have been erroneously removed). As observed in the motivating example, this minimum can become very small. A central idea of our proposed method Latent PCMCI (LPCMCI) is \(i\) to restrict the conditioning sets that need to be tested in the first place, and \(ii\) to extend those sets that are tested with additional conditions that increase effect size and at the same time do not induce spurious dependencies. While the latter demand is met by ancestors (see Lemma [S3]), the following theorem shows that adding known parents of \(X_{i \rightarrow r}\) and \(X_{j}^r\) as default conditions improves the effect size of LPCMCI over FCI, hence leading to higher recall. This generalizes the momentary conditional independence (MICI) [Runge et al., 2019b] idea to latent causal discovery and also holds in the non-time series case. We state the theorem in an information theoretic framework with \(I\) denoting (conditional) mutual information and \(I(X; Y; Z|W) = I(X; Y|W) - I(X; Y|W, Z)\) the interaction information (which is symmetric in its arguments before the “\(\mid\)”).

**Theorem 1** (LPCMCI effect size). Let \(X_{i \rightarrow r} \leftrightarrow X_{j}^r\) be a link (\(\rightarrow\) or \(\leftrightarrow\)) in \(\mathcal{M}(\mathcal{G})\). Denote the union of their parents without \(X_{i}^r\) and \(X_{j}^r\) themselves by \(\mathcal{P} = \{ \{X_{i \rightarrow r}, X_{j}^r\}, \mathcal{M}(\mathcal{G}) \} \setminus \{X_{i \rightarrow r}, X_{j}^r\}\) and the remaining variables by \(\mathcal{X}^* = \mathcal{X} \setminus \mathcal{P}\). Let \(S = \arg \min_{\hat{S} \subseteq \mathcal{X}^* \setminus \{X_{i \rightarrow r}, X_{j}^r\}} I(X_{i \rightarrow r}; X_{j}^r | \hat{S}, \mathcal{P})\) be the set of sets that define LPCMCI’s effect size. If there is \(S^* \in \hat{S}\) and a proper subset \(Q \subset \mathcal{P}\) such that \(S^* \subseteq \text{adj}(X_{i \rightarrow r}, \mathcal{M}(\mathcal{G})) \setminus \mathcal{P}\) or \(S^* \subseteq \text{adj}(X_{j}^r, \mathcal{M}(\mathcal{G})) \setminus \mathcal{P}\) and \(I(X_{i \rightarrow r}; X_{j}^r; \mathcal{P} \setminus Q | S^*, Q) < 0\), then

\[
\min_{\hat{S} \subseteq \mathcal{X}^* \setminus \{X_{i \rightarrow r}, X_{j}^r\}} I(X_{i \rightarrow r}; X_{j}^r | \hat{S}, \mathcal{P}) > \min_{\hat{S} \subseteq \mathcal{X}^* \setminus \{X_{i \rightarrow r}, X_{j}^r\}} I(X_{i \rightarrow r}; X_{j}^r | \hat{S}).
\]

(2)

If the assumptions are not fulfilled, then (trivially) "\(\geq\)" holds in (2).

The second assumption only requires that any subset of parents \(\mathcal{P}^* = \mathcal{P} \setminus Q \subseteq \mathcal{P}\) contains information that increases the information between \(X_{i \rightarrow r}\) and \(X_{j}^r\). Corollary [S1] details that a sufficient condition for this is the existence of any unshielded collider motif \(X_{i \rightarrow r} \leftrightarrow X_{j}^r \leftrightarrow \mathcal{P}^*\) together with additional assumptions (illustrated in Fig. [S1]) in particular that \(S^*\) should not contain descendants of \(X_{j}^r\).

This theorem leads to the following two guiding design principles behind LPCMCI. First, use known parents as default conditions. Second, do not test conditioning sets that contain known non-ancestors (which are unnecessary anyway according to Lemma [S5]). As additional benefit, there are fewer conditioning sets that need to be tested and hence a lower computational complexity. A disadvantage is the higher cardinality of conditioning sets. In [Runge et al., 2019b] it is discussed that conditioning on both parents also leads to better calibrated tests avoiding inflated false positives. To find parents and non-ancestors early on, we apply a novel set of orientation rules already during the skeleton discovery phase. We do not claim that our choice of default conditions is optimal, but our numerical experiments indicate strong increases in recall.
3.2 Introducing middle marks and LPCMCI-PAGs

To facilitate early orientation of edges we here give an unambiguous causal interpretation to the graph at every step of the algorithm. This is achieved by augmenting edges with middle marks. Since the discussion is independent of time order, we here and in the following section use generic variables $A$, $B$, and $C$.

Middle marks are denoted above the link symbol and can be ‘?’, ‘L’ , ‘R’, ‘!’, or ‘’ (empty). The ‘L’ (‘R’) on $A \xrightarrow{\bL \bL} B$ ($A \xleftarrow{\bL \bL} B$) asserts that if $A < B$ ($B < A$) then $B \notin \text{an}(A, G)$ or there is no $S \subseteq \text{pa}(A, M(G))$ that $m$-separates $A$ and $B$ in $M(G)$. Here $<$ is any total order on the set of variables. Its choice is arbitrary and does not influence the causal information content, the sole purpose being to disambiguate $A \xrightarrow{\bL \bL} B$ from $A \xleftarrow{\bL \bL} B$. Moreover, ‘∗’ is a wildcard that may stand for all three edge marks (tail, head, circle) that appear in PAGs. Further, the ‘!’ on $A \xrightarrow{\bL} B$ asserts that both $A \xrightarrow{\bL} B$ and $A \xleftarrow{\bL} B$ are true, and the empty middle mark on $A \xrightarrow{\bL} B$ says that $A \in \text{adj}(B, M(G))$. Lastly, the ‘?’ on $A \xrightarrow{\bL} B$ doesn’t promise anything. In all these cases non-circle edge marks, here potentially hidden by the ‘∗’, still convey their standard meaning of ancestorship and non-ancestorship.

We call a PAG $C(G)$ whose edges are extended with middle marks a LPCMCI-PAG for $M(G)$, see Sec. [S3] in the SM for a more formal definition. The ‘∗’ symbol is also used as a wildcard for the five middle marks, so $A \xrightarrow{\bL} B$ subsumes all possible edges.

Note that we are not changing the quantity we are trying to estimate, this is still the PAG $\mathcal{P}(G)$ as explained in Sec. [23]. The notion of LPCMCI-PAGs is used in intermediate steps of LPCMCI and is useful for two reasons. First, $A \xrightarrow{\bL} B$ is reserved for $A \in \text{adj}(B, M(G))$ and therefore has an unambiguous meaning at every point of the algorithm (unlike for FCI and RFCI). Second, middle marks carry fine-grained causal information that allows to determine definite adjacencies early on:

**Lemma 1** (Ancestor-parent-rule). In LPCMCI-PAG $C(G)$ one may replace 1.) $A \rightarrow B$ by $A \rightarrow B$, 2.) $A \rightarrow B$ for $A > B$ by $A \rightarrow B$, and 3.) $A \rightarrow B$ for $A < B$ by $A \rightarrow B$.

When LPCMCI has converged all middle marks are empty, then $C(G)$ is a PAG. We choose at total order consistent with time order, namely $X_i \xrightarrow{\tau} X_j$ iff $\tau > 0$ or $\tau = 0$ and $i < j$. Lagged links can then be initialized with edges $\xrightarrow{\tau}$ (contemporaneous links as $\xrightarrow{\tau}$).

3.3 Orientations rules for LPCMCI-PAGs

We now discuss rules for edge orientation in LPCMCI-PAGs. For this we need a definition:

**Definition 1** (Weakly minimal separating sets). In MAG $M(G)$ let $A$ and $B$ be $m$-separated by $S$. The set $S$ is a weakly minimal separating set of $A$ and $B$ if i) it decomposes as $S = S_1 \cup S_2$ with $S_1 \subseteq \text{an}(\{A, B\}, M(G))$ such that ii) if $S' = S_1 \cup S_2'$ with $S_2' \subseteq S_2$ $m$-separates $A$ and $B$ then $S_2' = S_2$. The pair $(S_1, S_2)$ is called a weakly minimal decomposition of $S$.

This generalizes the notion of minimal separating sets, for which additionally $S_1 = \emptyset$. Since LPCMCI is designed to extend conditioning sets by known ancestors, the separating sets it finds will in general not be minimal but still be weakly minimal. The following Lemma, a generalization of the unshielded triple rule [Colombo et al., 2012], is central to orientations in LPCMCI-PAGs:

**Lemma 2** (Strong unshielded triple rule). Let $A \xrightarrow{\bL} B \xrightarrow{\bL} C$ be an unshielded triple in LPCMCI-PAG $C(G)$ and $S_{AC}$ the separating set of $A$ and $C$. 1.) If i) $B \in S_{AC}$ and ii) $S_{AC}$ is weakly minimal, then $B \in \text{an}(\{A, C\}, G)$. 2.) Let $T_{AB} \subseteq \text{an}(\{A, B\}, M(G))$ and $T_{CB} \subseteq \text{an}(\{C, B\}, M(G))$ be arbitrary. If i) $B \notin S_{AC}$, ii) $A$ and $B$ are not $m$-separated by $S_{AC} \cup T_{AB} \setminus \{A, B\}$, iii) $C$ and $B$ are not $m$-separated by $S_{AC} \cup T_{CB} \setminus \{C, B\}$, then $B \notin \text{an}(\{A, C\}, G)$. The conditioning sets in ii) and iii) may be intersected with the past and present of the later variable.

Part 2.) of this Lemma generalizes the FCI collider rule $R_0$ to rule $R_0'$ (of which there are several variations when restricting to particular middle marks), and part 1.) generalizes $R_1$ to $R_1'$. Rules $R_2$ and $R_8$ generalize trivially to triangles in $C(G)$ with arbitrary middle marks, giving rise to $R_2'$ and $R_8'$. Rules $R_3$, $R_9$ and $R_{10}$ are generalized to $R_3'$, $R_9'$ and $R_{10}'$ by adding the requirement that the middle variables of certain unshielded colliders be in the separating set of the two outer variables, and that these separating sets be weakly minimal. Since there are no selection variables, rules $R_5$, $R_6$ and $R_7$ are not applicable. Rule $R_4'$ is a generalization of the discriminating path rule [Colombo et al., 2012] of RFCI. These rules are complemented by the replacements specified in Lemma [1]. Precise formulations of all rules are given in Sec. [S4] of the SM.
We stress that these rules are applicable at every point of the algorithm and that they may be executed in any order. Soundness of the FCI orientation phase requires that prior to orientation a PAG has been found. Also RFCI orients only once an RFCI-PAG has been determined. Both FCI and RFCI require that all colliders be oriented first.

### 3.4 The LPCMCI algorithm

LPCMCI is a constraint-based causal discovery algorithm that utilizes the findings of Sec. 3.1 to increase the effect size of CI tests. High-level pseudocode is given in Algorithm 1. After initializing \( \mathcal{C}(G) \) as a complete graph, the algorithm enters its preliminary phase in lines 2 to 4. This involves calls to Algorithm S2 (pseudocode in Sec. S5 of the SM), which removes many (but in general not all) wrong edges and, while doing so, repeatedly applies orientation rules. These rule will identify a subset of the (non-)ancestorships in \( G \) and mark them by heads or tails on edges in \( \mathcal{C}(G) \). The non-ancestorships are used to further constrain the conditioning sets \( S \) of subsequent CI test, the ancestorships to extend these sets \( S \rightarrow S \cup S_{\text{def}} \) with \( S_{\text{def}} = pa(A_{\text{def}}) = \rho(\{X_{t-\tau}, X_{t-l}\}, C(G)) \) denoting the known parents of those variables whose independence is being tested. All parentships marked in \( \mathcal{C}(G) \) after line 3 are remembered and carried over to an elsewise re-initialized purpose of this iterative process is to determine an accurate subset of the parentships in \( G \), which are then passed on to the final phase in lines 5 - 6. Algorithm S2 may not remove edges between some pairs of non-adjacent variables for which neither one of them is ancestor of the other. This is the purpose of Algorithm S3 (pseudocode in Sec. S5 of the SM) that is called in line 6 (this is similar to FCI’s second removal phase). Algorithm S3 repeatedly applies orientation rules and uses identified (non-)ancestorships in the same way as Alg. S2. As stated in the following theorems, LPCMCI will then have found the PAG \( \mathcal{P}(G) \). Moreover, its output does not depend on the order of the \( N \) time series variables \( X^j \). The number \( k \) of iterations in the preliminary phase is a hyperparameter, we write LPCMCI(\( k = k_0 \)) when specifying \( k = k_0 \). Stationarity, both for orientations and adjacencies, is enforced at every step of the algorithm.

#### Algorithm 1 LPCMCI

**Require**: Time series dataset \( X = \{X^1, \ldots, X^N\} \), maximal considered time lag \( \tau_{\text{max}} \), significance level \( \alpha \), CI test CI(\( X, Y, S \)), non-negative integer \( k \)

1: Initialize \( \mathcal{C}(G) \) as complete graph with \( X^i_{t-\tau} \leftrightarrow X^i_{t} \) (\( 0 < \tau \leq \tau_{\text{max}} \)) and \( X^i_{t-\tau} \leftrightarrow \circ \circ X^j_{t} \) (\( \tau = 0 \))
2: for \( 0 \leq l \leq k - 1 \) do
3: Remove edges and apply orientations using Algorithm S2
4: Repeat line 1, orient edges as \( X^i_{t-\tau} \rightarrow X^j_{t} \) if \( X^i_{t-\tau} \rightarrow X^j_{t} \) was in \( \mathcal{C}(G) \) after line 3
5: Remove edges and apply orientations using Algorithm S2
6: Remove edges and apply orientations using Algorithm S3
7: return PAG \( \mathcal{C}(G) = \mathcal{P}(G) = \mathcal{P}(G)_{\tau_{\text{max}}}^{\text{statAO}} \)

**Theorem 2** (LPCMCI is sound and complete). Assume that there is a process as in eq. (1) without causal cycles, which generates a distribution \( P \) that is faithful to its time series graph \( G \). Further assume that there are no selection variables, and that we are given perfect statistical decisions about CI in the marginal of \( P \). Then LPCMCI is sound and complete, i.e., it returns the PAG \( \mathcal{P}(G) \).

**Theorem 3** (LPCMCI is order-independent). The output of LPCMCI does not depend on the order of the \( N \) time series variables \( X^j \) (the \( j \)-indices may be permuted).

### 3.5 Back to the motivational example in Fig. 1

The first iteration \( (l = 0) \) of LPCMCI also misses the links \( Y_{t-1} \rightarrow Z_t \) and finds \( X_{t} \rightarrow Y_{t} \) in only few realizations (we here suppress middle marks for simpler notation), but orientations are already improved as compared to FCI. Rule R1′ applied after \( p = 1 \) orients the auto-links \( X_{t-1} \rightarrow X_t \) and \( Y_{t-1} \rightarrow Y_t \). This leads to the parents sets \( pa(X_t, \mathcal{C}(G)) = \{X_{t-1}\} \) and \( pa(Y_t, \mathcal{C}(G)) = \{Y_{t-1}\} \), which are then used as default conditions in subsequent CI tests. This is relevant for orientation rule R0′ that tests whether the middle node of the unshielded triple \( X_{t-1} \leadsto Y_t \leadsto Y_{t} \) does not lie in the separating set of \( X_{t-1} \) and \( Y_t \). Due to the extra conditions the relevant partial correlation \( \rho(X_{t-1}; Y_t|X_t, X_{t-2}, Y_{t-1}) \) now correctly turns out significant. This identifies \( X_t \) as collider and
We here compare FCI, RFCI and LPCMCI with CI tests based on linear partial correlation (ParCorr), results for the nonparametric GPDC test [Runge et al., 2019b] are given in the SM. To limit runtime, we constrain the cardinality of conditioning sets to 3 in the second removal phase of FCI and in Alg. S3 of LPCMCI (excluding default conditions). We generate datasets with this variant of SCM (1):

$$V_j^t = a_j V_j^{t-1} + \sum_i c_i f_i(V_i^{t-\tau_i}) + \eta_j^t \quad \text{for } j \in \{1, \ldots, \tilde{N}\}$$  \hspace{1cm} (3)

Autocorrelations $a_j$ are uniformly drawn from $[\max(0, a - 0.3), a]$ for some $a$ as indicated in Fig. 2 and $\eta_j^t \sim \mathcal{N}(0, \sigma_j^2)$ is iid with $\sigma_j$ drawn from $[0.5, 2]$. In addition to autocorrelation links, we randomly choose $L = \tilde{N}$ linear cross-links for each model (see nonlinear $f_i$ with non-Gaussian noise in SM). The coefficients $c_i$ are drawn uniformly from $[-0.2, 0.8]$. 30% of the links are contemporaneous ($\tau_i = 0$), the remaining $\tau_i$ are drawn from $[1, p_{\text{ts}} = 3]$. We only consider stationary models. From the $\tilde{N}$ variables of each dataset we randomly choose $\lambda = 30\%$ as unobserved and denote the number of observed variables as $N$. As discussed in Sec. 2.3, the true PAG $\mathcal{P}(\mathcal{G})$ of each model depends on the $\tau_{\text{max}}$ chosen. In Fig. 2 we show the relative average numbers of directed, bidirected, and (partially) unoriented links. For performance evaluation true positive (= recall) and false positive rates for adjacencies are distinguished between lagged cross-links ($i \neq j$), contemporaneous, and autodependency links. False positives instead of precision are shown to investigate whether methods can control these below the $\alpha$-level. Orientation performance is
evaluated based on edgemark recall and precision. In Fig. 2, we also show the average of minimum absolute ParCorr values as an estimate of effect size and the maximum cardinality for each true link over all CI tests in the respective methods. All metrics are computed across all estimated graphs from 500 realizations of the model in eq. (3) at time series length $T$. The average (and std.) runtime estimates were evaluated on Intel Xeon Platinum 8260.

In Fig. 2A, we show LPCMCI for $k = 0, \ldots, 4$ against increasing autocorrelation $a$. Note that $a = 0$ implies a different true PAG than $a > 0$. The largest gain, both in recall and precision, comes already from $k = 0$ to $k = 1$. For higher $k$ LPCMCI maintains false positive control and orientation precision, and improves recall before converging at $k = 4$. The gain in recall is largely attributable to improved effect size. On the downside, larger $k$ increase cardinality (estimation dimension) and runtime. However, the runtime increase is only marginal because later $l$-steps converge faster and the implementation caches CI test results. In Fig. 2B we show the comparison of LPCMCI with FCI and RFCI against autocorrelation, depicting LPCMCI for $k = 0$ and $k = 4$. Already LPCMCI($k = 0$) has higher adjacency and orientation recall than FCI and RFCI for increasing autocorrelation while they are on par for $a = 0$. This comes at the price of precision, especially lagged orientation precision. LPCMCI($k = 4$) then has more than 0.5 higher contemporaneous orientation recall and still 0.1 higher lagged orientation recall than FCI and RFCI. Lagged precision is higher for high autocorrelation and contemporaneous precision is slightly lower. LPCMCI($k = 4$) maintains high recall for increasing autocorrelation $a \geq 0.5$ while FCI and RFCI’s recall sharply drops. These results can be explained by improved effect size while the increased cardinality ($\approx 5$) of separating sets is still moderate compared to the sample size $T = 500$. LPCMCI($k = 0$) has similar low runtime as RFCI, for LPCMCI($k = 4$) it is comparable to that of FCI. In Fig. 2C, we show results for different numbers of variables $N$. As expected, all methods have decreasing adjacency and orientation recall for higher $N$, but LPCMCI starts at a much higher level. For $N = 3$ both FCI and RFCI cannot control false positives for lagged links while for larger $N$ false positives become controlled. The reason is the interplay of ill-calibrated CI tests for smaller $N$ (inflating false positives) with sequential testing for larger $N$ (reducing false positives), as has been discussed in [Runge et al., 2019b] for the similar PC algorithm [Spirtes and Glymour, 1991]. LPCMCI better controls false positives here, its decreasing recall can be explained by decreasing effect size and increasing cardinality. Runtime becomes slightly larger than that of FCI for larger $N$. In Fig. 2D we show results for different maximum time lags $\tau_{max}$. Note that these imply different true PAGs, especially since further lagged links appear for larger $\tau_{max}$. All methods show a decrease in lagged recall and precision, whereas contemporaneous recall and precision stays almost constant. For FCI there is an explosion of runtime for higher $\tau_{max}$, the reason being excessive searches of separating sets in its second removal phase. In LPCMCI this is partially overcome since the sets that need to be searched through are more restricted. Results for further combinations of model parameters $N, a, \lambda, T$ and method parameters $\alpha, k$ are shown in Sec. [S8]. In the nonlinear case, where all methods are run with the GPDC CI test [Runge et al., 2019b], LPCMCI has higher precision than FCI and RFCI.

5 Discussion and future work

Major strengths of LPCMCI lie in its significantly improved recall as compared to the FCI and RFCI baselines, which grows with autocorrelation and is particularly strong for contemporaneous links. At the same time LPCMCI (for $k > 0$) controls false positive adjacencies better than the baselines. We cannot prove false positive control, but are not aware of any such proof for other constraint-based algorithms in the challenging latent, non-linear, autocorrelated setting considered here. A general weakness, which also applies to FCI and RFCI, is the faithfulness assumption. This may be violated in practice and then lead to wrong conclusions. Moreover, like all constraint-based methods, our method cannot distinguish different members of Markov equivalence classes like methods based on the SCM framework such as e.g. TS-LiNGAM [Hyvärinen et al., 2008] and TIMINO [Peters et al., 2013] do. These, on the other hand, restrict the type of dependences. Concluding, this paper shows how causal discovery in autocorrelated time series benefits from increasing the effect size of CI tests by including known causal parents in conditioning sets. The LPCMCI algorithm introduced here implements this idea by entangling the removal and orientation of edges. As demonstrated in extensive simulation studies, LPCMCI achieves much higher recall than the FCI and RFCI baselines. The construction of LPCMCI moreover involves novel orientation rules and an extension of graphical terminology by the notions of middle marks and weakly minimal separating sets. Code for all studied methods is
provided. In future work one may relax assumptions of LPCMCI to allow for selection bias and non-stationarity. It would also be interesting to combine the ideas presented here with the structural causal model framework. Another question is whether one can define limiting time series MAGs and PAGs regarding the maximum time lag.
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Supplementary material

In this supplementary material we present a brief overview of the FCI algorithm and related graphical terminology as well as details, proofs, and further simulation studies that have been omitted from the main text for reasons of space.

We always assume that there are no selection variables. When saying that $S$ (also known as full time graph) using generic names does not imply The Markov equivalence class of a MAG is the set of all MAGs that yield the exact same set of

The structural causal model (SCM) in eq. (1) can be graphically represented by its time series graph

is a notational device only, there are no ' equivalence class in which there is a tail instead and some other member in which there is a head

maximally informative is further said to be

is a PAG for MAG

pa spouses) of the individual variables. Example:

adjacencies, spouses) of a set of variables are defined as the union of parents (ancestors, adjacencies, spouses) of the individual variables. Example:

In the presence of unobserved variables so called maximal ancestral graphs (MAGs)

provide an appropriate graphical language for representing causal relationships. Since in this paper we assume the absence of selection variables, the relevant MAGs $M$ contain two types of edges: directed ‘$\rightarrow$’ and bidirected ‘$\leftrightarrow$’. These edges are interpreted as composite objects constituted by the symbols at their ends (edge marks), which can be an (arrow-)head (‘$>$’ or ‘$<$’) or a tail (‘$\cdot$’). These edge marks carry a causal meaning: Tails convey ancestorships in $G$, i.e., $X_{i-\tau}$ $\rightarrow$ $X_i$ in $M$ asserts that $X_i \in an(X_i, G)$; heads convey non-ancestorships in $G$, i.e., $X_{i-\tau}$ $\rightarrow$ $X_i$ and $X_i \leftrightarrow$ $X_i$ in $M$ say that $X_i \notin an(X_i, G)$. As an immediate consequence of time order there cannot be a link $X_{i-\tau} \leftarrow X_i$ for $\tau > 0$ (an effect cannot precede its cause). Parents, ancestors and adjacencies are defined in the same way as for DAGs, and the spouses $sp(X_i, M)$ of $X_i$ are the set of nodes $X_{i-\tau}$ with $X_{i-\tau}$ $\leftrightarrow$ $X_i$ in $M$. Two variables are connected by an edge in $M$ if and only if they cannot be d-separated by a subset of observed variables in $G$, and d-separation in $G$ restricted to observed variables is equivalent to m-separation in $M$ [Pearl, 1988, Verma and Pearl, 1990, Richardson and Spirtes, 2002]. The parents (ancestors, adjacencies, spouses) of a set of variables are defined as the union of parents (ancestors, adjacencies, spouses) of the individual variables. Example: $pa(\{A, B\}, \cdot) = pa(A, \cdot) \cup pa(B, \cdot)$.

The Markov equivalence class of a MAG is the set of all MAGs that yield the exact same set of m-separations [Zhang, 2008]. These are graphically represented by partial ancestral graphs (PAGs), in which the set of allowed edge marks is extended by the circle mark ‘$\cdot$’ [Zhang, 2008]. Such a graph is said to be a PAG for MAG $M$ if i) it has the same nodes and adjacencies as $M$ and if ii) all its non-circle edge marks are shared by all members in the Markov equivalence class of $M$. It is further said to be maximally informative if for all its circle marks there is some member of the equivalence class in which there is a tail instead and some other member in which there is a head instead. The wildcard symbol ‘$*$’ may stand for all three possible edge marks (head, tail, circle). This is a notational device only, there are no ‘$*$’ marks in PAGs.

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S2 Some background on FCI

The Fast Causal Inference (FCI) algorithm is an algorithm for constraint-based causal discovery in the presence of unobserved variables [Spirtes et al., 1995, 2000, Zhang, 2008]. It allows for both latent confounders and selection variables, although in this paper we assume the absence of selection variables. Under the assumptions of faithfulness [Spirtes et al., 2000], acyclicity, and the existence of an underlying SCM the algorithm determines the maximally informative PAG from perfect statistical decisions of conditional independencies in the distribution $P$ generated by the SCM. The algorithm is based on the following fact:

**Proposition S1** (m-separation by subsets of D-Sep sets [Spirtes et al., 2000]). Let $A$ and $B$ be two nodes such that $A \notin adj(B, M)$ and $B \notin an(A, M)$, then they are m-separated by some subset of $D-Sep(B, A, M)$. Here:

**Definition S2** (D-Sep sets [Spirtes et al., 2000]). Node $V$ is in $D-Sep(B, A, M)$ if and only if $i$) it is not $B$ and $ii$) there is a path $p_V$ such that $iia)$ all nodes on $p_V$ are in $an\{A, B\}$, $M$ and $iib)$ all non end-point nodes on $p_V$ are colliders on $p_V$.

A node $B$ is a collider on a path $p$ if the two edges on $p$ involving $B$ both have a head at $B$, as e.g. in $A \rightarrow B \leftarrow C$, otherwise in it is a non-collider. Together with acyclicity Proposition S1 guarantees that non-adjacent variables $A$ and $B$ are m-separated by a subset of $D-Sep(B, A, M)$ or a subset of $D-Sep(A, B, M)$. However, $M$ is initially unknown and the D-Sep sets cannot be determined without prior work. Therefore, starting from the complete graph over the set of variables, FCI first performs test of CI given subset of $pa(B, M')$ and $pa(A, M')$ where $M'$ is the (changing) graph that the algorithm operates on. Whenever two variables are found to be conditionally independent given some subset of variables, the edge between them is removed and their separating set is remembered. This removes some, but in general not all false links. Second, the algorithm orients all resulting unshielded triples $A \leftrightarrow B \leftrightarrow C$ in $M$ as colliders $A \leftrightarrow B \leftrightarrow C$ if $B$ is not in the separating set of $A$ and $C$ (rule $R0$). We note that at this point head marks are not guaranteed to convey non-ancestorships, but those unshielded triples that are part of $M$ are oriented correctly. This is enough to determine the Possible-D-Sep sets, see [Spirtes et al., 2000], which are supersets of the D-Sep sets define above. Third, FCI performs test of CI given subsets of Possible-D-Sep($B, A, M'$) and Possible-D-Sep($A, B, M'$). This removes all false links. Fourth, all previous orientations are undone, $R0$ is applied once more and then followed by exhaustive application of the ten rules $R1$ through $R10$. Test of CI are preferentially made given smaller conditioning sets $S$, i.e., FCI first tests sets with $|S| = p = 0$, then those with $|S| = p = 1$ and so on.

S3 LPCMCI-PAGs

Section 3.2 introduced middle marks and LPCMCI-PAGs. We here give a more formal definition of these notions. Recall that we assume the absence of selection variables.

**Definition S3** (LPCMCI-PAGs). Consider a simple graph $C(G)$ over the same set of variables as $M(G)$ with edges of the type $\rightarrow$, $\leftrightarrow$, $\diamondsuit$, and $\odot$ where the wildcard ‘$*$’ can stand for the five possible middle marks ‘?”’, ‘’’, ‘’’, ‘!’, or ‘’’’’ (empty). Such $C(G)$ is a LPCMCI-PAG for $G$ with respect to total order $<$ for any probability distribution $P$ that is Markov relative and faithful to $G$ the following seven conditions hold:

1. If $A \leftrightarrow B$ in $C(G)$, then $B \notin an(A, G)$.
2. If $A \rightarrow B$ in $C(G)$, then $A \in an(B, G)$.
3. If $A \notin adj(B, C(G))$, then $A \notin adj(B, M(G))$.
4. If $A \leftrightarrow B$ in $C(G)$ for $A < B$, then $B \notin an(A, G)$ or there is no $S \subseteq pa(A, M(G))$ that m-separates $A$ and $B$ in $M(G)$.
5. If $A \leftrightarrow B$ in $C(G)$ for $A < B$, then $A \notin an(B, G)$ or there is no $S \subseteq pa(B, M(G))$ that m-separates $A$ and $B$ in $M(G)$.
6. If $A \leftarrow B$ in $C(G)$, then both $A \leftrightarrow B$ and $A \leftrightarrow B$ would be correct.
7. If $A \rightarrow B$ in $C(G)$, then $B \in adj(A, M(G))$. 

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The first two points give the same causal meaning to head and tail edge marks as they have in MAGs and PAGs. We repeat that while this definition involves of a fixed total order $<$, its choice is arbitrary and without influence on the conveyed causal information. Moreover, the definition does not depend on time order. Also note that if all middle marks in $C(G)$ are empty, then $C(G)$ is a PAG for $M(G)$ (guaranteed by the first, second, third, and seventh point). Parents, ancestors, descendants, spouses, and adjacencies in $C(G)$ are defined (and denoted) in the same way as for MAGs and PAGs, i.e., without being influenced by middle marks.

### S4 Orientation rules for LPCMCI-PAGs

The following is a list of rules for orienting edges in LPCMCI-PAGs. These are extensions of the standard FCI rules [Zhang, 2008] as well as the unshielded triple rule and discriminating path rule of RFCI [Colombo et al., 2012]. If a rule proposes to orient the same edge mark as both tail and head, this is resolved by putting a conflict mark ‘x’ instead. The edge mark wildcard ‘*’ is redefined to stand for the circle, head, tail or conflict mark; the second wildcard symbol ‘*’ excludes the conflict mark. For two reasons we explicitly present and prove also those rules that generalize without much modification: To demonstrate their validity for LPCMCI-PAGs, and to show in which cases the rules also apply to structures with conflict marks.

If $X \rightarrow Y \rightarrow Z$ is an unshielded triple we write $S_{XZ}$ for the separating set of $X$ and $Z$. Many rules require that $S_{XZ}$ be weakly minimal and $Y \in S_{XZ}$. In all these cases the requirement of weak minimality can be dropped if $X \rightarrow Y \rightarrow Z$, i.e., if both middle marks on $X \rightarrow Y \rightarrow Z$ are empty. For this reason the standard FCI orientation rules are implied as special cases.

**R0**a: For all unshielded triples $A \rightarrow B \leftarrow C$: If $ia)$ $A \rightarrow B$ or $ib)$ $A$ and $B$ are conditionally dependent given $S\cup\{A, B, C(G)\}$ \ $\{A, B, C, B\}$, then mark the edge between $A$ and $B$ for orientation as collider $A \rightarrow B \leftarrow C$. Condition $ib)$ need only be checked if not $ia)$, and $iia)$ need only be checked if not $iia)$, and $iia)$ need only be checked if all previous conditions are true. If $iia)$ or $iia)$ find a conditional independence, mark the corresponding edge(s) for removal.

**R0**b: For all unshielded triples $A \rightarrow B \leftarrow C$ and for all unshielded triples $A \rightarrow B \leftarrow C$ with $B < C$ and for all unshielded triples $A \rightarrow B \leftarrow C$ with $B > C$: If $ia)$ $A \rightarrow B$ or $ib)$ $A$ and $B$ are conditionally dependent given $S\cup\{A, B, C(G)\}$ \ $\{A, B, C, B\}$, then mark the edge between $A$ and $B$ or orientation as $B \leftarrow C$ (the middle mark remains as it was before). Condition $ib)$ need only be checked if not $ia)$, and $iib)$ need only be checked if all previous conditions are true. If $iib)$ finds a conditional independence, mark the corresponding edge for removal.

**R0**c: For all unshielded triples $A \rightarrow B \leftarrow C$ and for all unshielded triples $A \rightarrow B \leftarrow C$ with $B < C$ and for all unshielded triples $A \rightarrow B \leftarrow C$ with $B > C$: If $B \notin S_{AC}$, then mark the edge between $B$ and $C$ for orientation as $B \leftarrow C$ (the middle mark remains as it was before).

**R0**d: For all unshielded triples $A \rightarrow B \leftarrow C$ and for all unshielded triples $A \rightarrow B \leftarrow C$: If $B \notin S_{AC}$, then mark the edge between $B$ and $C$ for orientation as $B \leftarrow C$ (the middle mark remains as it was before).

**R1**: For all unshielded triples $A \rightarrow B \leftarrow C$: If $S_{AC}$ is weakly minimal and $B \in S_{AC}$, then mark the edge between $B$ and $C$ for orientation as collider $A \rightarrow B \leftarrow C$.

**R2**: For all $A \rightarrow B \leftarrow C$ with $A \leftarrow C$ and for all $A \rightarrow B \leftarrow C$ with $A \leftarrow C$: Mark the edge between $A$ and $C$ for orientation as $A \rightarrow C$.

**R3**: For all unshielded triples $A \rightarrow B \leftarrow C$ with $A \leftarrow D \leftarrow C$ and $D \leftarrow B$: If $S_{AC}$ is weakly minimal and $D \in S_{AC}$, then mark the edge between $D$ and $B$ for orientation as $D \leftarrow B$.

**R4**: Use the discriminating path rule of [Colombo et al., 2012] with the following modification: When the rule instructs to test whether any pair $(A, B)$ of variables is conditionally independent given any set $S$, then $i)$ if $A$ and $B$ are connected by an edge with empty middle mark do not test this, and $ii)$ else replace $S$ with $S \cup \{A, B, C(G)\}$ \ $\{A, B, C, B\}$, nodes in the future of both $A$ and $B$.

**R8**: For all $A \rightarrow B \rightarrow C$ with $A \leftarrow C$: Mark the edge between $A$ and $C$ for orientation as $A \rightarrow C$.
Algorithm S2

\textbf{Require:} LPCMCI-PAG $C(G)$, memory of minimal test statistic values $I_{\text{min}}^{\text{lag}}(\cdot, \cdot)$, memory of separating sets $\text{SepSet}(\cdot, \cdot)$, time series dataset $X = \{X^1, \ldots, X^N\}$, maximal considered time lag $\tau_{\text{max}}$, significance level $\alpha$, CI test CI($X$, $Y$, $S$)

1: repeat starting with $p = 0$
2: \hspace{1em} for $-1 \leq m \leq \tau_{\text{max}}$
3: \hspace{2em} for all ordered pairs of variables $(X^i_{t\rightarrow r}, X^j_t)$ adjacent in $C(G)$ with $X^i_{t\rightarrow r} < X^j_t$
4: \hspace{3em} if $(m = -1$ and $i \neq j)$ or $(m \geq 0$ and $r \neq m$ or $i = j)$ then continue with next pair
5: \hspace{3em} $S_{\text{def}} = pa(\{X^i_{t\rightarrow r}, X^j_t\}, C(G))$
6: \hspace{3em} if the middle mark is ‘? ’ or ‘L’ then
7: \hspace{4em} $S_{\text{search}} = \text{apds}_{s_1}(X^i_{t\rightarrow r}, X^j_t, C(G)) \setminus S_{\text{def}}$, ordered according to $I_{\text{min}}^{\text{lag}}(X^i_{t\rightarrow r}, \cdot)$
8: \hspace{3em} if $|S_{\text{search}}| < p$ then update middle mark with ‘R’ according to Lemma S8
9: \hspace{3em} for all subsets $S \subseteq S_{\text{search}}$ with $|S| = p$
10: \hspace{4em} $(p$-value, $I) \leftarrow \text{CI}(X^i_{t\rightarrow r}, X^j_t, S \cup S_{\text{def}})$
11: \hspace{4em} $I_{\text{min}}^{\text{lag}}(X^i_{t\rightarrow r}, X^j_t) = I_{\text{min}}^{\text{lag}}(X^i_{t\rightarrow r}, X^j_t) = \min(|I|, I_{\text{min}}^{\text{lag}}(X^i_{t\rightarrow r}, X^j_t))$
12: \hspace{4em} if $p$-value $> \alpha$ then
13: \hspace{5em} mark edge for removal, add $S \cup S_{\text{def}}$ to SepSet$(X^i_{t\rightarrow r}, X^j_t)$
14: \hspace{5em} break innermost for-loop
15: \hspace{3em} repeat lines 6 - 14 with $X^i_{t\rightarrow r}$ and $X^j_t$ as well as ‘R’ and ‘L’ swapped
16: remove all edges that are marked for removal from $C(G)$
17: if any edge has been removed in line 16 then
18: run Alg. S4 using [APR, MMR, R8', R2', R1', R0', R0'1'], orient lagged links only
19: let $p = 0$
20: else increase $p$ to $p + 1$
21: until there are no other middle marks than ‘!’ or ‘ ’ (empty)
22: run Alg. S4 using [APR, MMR, R8', R2', R1', R0'd, R0'e, R3', R4, R9', R10', R0'b, R0'a]
23: return $C(G)$, $I_{\text{min}}^{\text{lag}}(\cdot, \cdot)$, SepSet$(\cdot, \cdot)$

Algorithm S2 removes the edges between all pairs $(X^i_{t\rightarrow r}, X^j_t)$ of variables that are not adjacent in $\mathcal{M}(G)$ and for which one of them is an ancestor of the other (it may also removed edges between some
pairs of non-adjacent variables for which neither one of them is ancestor of the other, but this is not guaranteed. To this end the algorithm tests for CI given $S \cup S_{\text{def}}$, where the cardinality $|S| = p$ of $S \subseteq S_{\text{search}} = \text{apds}_t(S(X^i_t),X^i_{t-\tau},C(G)) \setminus S_{\text{def}}$ is successively increased. The $\text{apds}_t$ sets are defined in Sec. 5 below, they exclude all variables that have already been identified as non-ancestors of $X^i_t$. This reflects the second design principle behind LPCMCI, see Sect. 3.1. The default conditioning set $S_{\text{def}} = \text{pa}(X^i_t),C(G)$ consists of all variables that have been marked as parents of $X^i_{t-\tau}$ or $X^i_t$ in $C(G)$, which implies that they are ancestors of $X^i_{t-\tau}$ or $X^i_t$ in $G$. The extension of $S$ to $S \cup S_{\text{def}}$ reflects the first design principle behind LPCMCI, see Sect. 3.1 and according to Lemma 5.4 cannot destroy m-separations. The parentships used to define $S_{\text{def}}$ are found by the application of orientation rules in line 18 (with Alg. 5.4 see further below in this section) that are made if at least one edge was removed in the current step of the repeat-loop (or have been passed on from an earlier iteration in the preliminary phase of LPCMCI). It is then necessary to restart with $p = 0$, otherwise future separating sets might not be weakly minimal. The rules may also find non-ancestorships, these then further restrict the $\text{apds}_t$ sets. Another novelty is that some edges are tested and removed (if found insignificant) before other edges are tested, see lines 2, 4 and the indentation of line 16. To be precise: All autodependency links are tested first, followed by cross links starting with lag $\tau = 0$ and moving to lag $\tau = \tau_{\text{max}}$ in steps of one. This ordering does not depend on the ordering of the $N$ time series variables $X^j$ and does therefore not introduce order-dependence in the sense studied in [Colombo and Maathuis, 2014]. The algorithm converges once all middle marks in $C(G)$ are ‘!’ or empty. By means of the APR rule (see Lemma 4 or Sect. 5.4) all edges with a tail mark will then have an empty middle mark, i.e., they cannot be $m$-separated and do not need further testing. Line 11 updates a memory for keeping track of the minimum test statistic value across all previous CI tests for a given pair of variables (the memory is initialized to plus infinity when line 1 of Algorithm 4 is executed). These values are used to sort $S_{\text{search}}$ in line 7 such that $X^i_{t-\tau}$ in $S_{\text{search}}$ if $I_{\min}(X^i_t,X^i_{t-\tau}) > I_{\min}(X^i_t,X^i_{t-\tau})$. Note that in line 18 only a select subset of rules is applied and that these are only used to orient lagged links. Moreover, in line 22 we choose to apply the standard rule $R4$ rather than the modified rule $R4'$. The reason for this is that, as observed in [Colombo and Maathuis, 2014], the discriminating path rule (on which $R4'$ is based) becomes computationally intensive when applied in an order-independent way involving conflict resolution. We found these choices to work well in practice but do not claim their optimality.

Algorithm 5.4 is structurally similar to Algorithm 5.2. Once called in line 6 of Algorithm 5.2 all middle marks in $C(G)$ are ‘!’ or empty. Whereas edges with empty middle mark are in $M(G)$ for sure, some edges with middle mark ‘!’ might not be in $M(G)$. Those latter type of edges are between pairs of variables in which neither one of them is ancestor of the other. According to Lemma 5.3 below in combination with Proposition 5.1 such pairs are $m$-separated by some subset of $\text{napds}_t(X^i_t,X^i_{t-\tau},C(G))$ as well as by some subset of $\text{napds}_t(X^i_{t-\tau},X^i_t,C(G))$. These sets are defined in Sec. 5.5 below, they are the more restricted LPCMCI equivalent of the Possible-D-Sep sets in FCI and the $\text{pds}_t$ sets in SVAR-FCI. For computational reasons the algorithm nevertheless only searches for separating sets in $\text{napds}_t(S(X^i_t),X^i_{t-\tau},C(G))$, unless for $\tau = 0$ where order-independence dictates otherwise. This is the reason for the logical or-connection in line 10. As compared to Algorithm 5.2 the default conditioning is extended: According Definition 5.3 a tail on an edge in $C(G)$ signifies ancestorship in $G$. Since $C(G)$ is an LPCMCI-PAG at every point of LPCMCI, $X^i_{t-\tau}$ is an ancestor of $X^i_t$ if there ever was the link $X^i_{t-\tau} \rightarrow X^i_t$. This gives rise to the set $S_{\text{def}}^2$ in line 6. In addition to the parents in $C(G)$, the algorithm also conditions per default on all nodes in $S_{\text{def}}^2$ that are in the current $\text{napds}_t$ set. This decreases the number of sets $S$ that need to be searched through in the for-loop in line 12 at the price of a higher-dimensional conditioning set. Also extended default conditioning cannot destroy $m$-separations. Non-ancestorships are used to constrain the $\text{napds}_t$ sets in the first place, and prior to determining $\text{napds}_t$ sets the collider rule $R0\prime$ a must have been applied to all unshielded triples in $C(G)$. The algorithm converges once all middle marks are empty, followed by a final exhaustive rule application to guarantee completeness.

Algorithm 5.4 exhaustively applies a given set of orientation rules specified by an ordered list $r$. The rules are executed in this order and, once any rule has modified $C(G)$, the loop jumps back to the first rule. This can be used for a preferential execution of simpler and less time consuming rules. Rules $R0\prime a$ and $R0\prime b$ involve CI tests and may therefore remove some edges. The corresponding separating set are not guaranteed to be weakly minimal, see Example 1 in the supplement paper to [Colombo et al., 2012] for a counterexample. (There this example is used to show that the separating
Algorithm S3 Non-ancestral removal phase

Require: LPCMCI-PAG \( C(G) \), memory of minimal test statistic values \( I_{\min}(\cdot, \cdot) \), memory of separating sets \( \text{SepSet}(\cdot, \cdot) \), time series dataset \( X = \{X_1, \ldots, X_N\} \), maximal considered time lag \( \tau_{\max} \), significance level \( \alpha \), CI test \( \text{CI}(X, Y, S) \)

1: repeat starting with \( p = 0 \)
2: for \(-1 \leq m \leq \tau_{\max}\) do
3: for all ordered pairs of variables \( (X_{i_{m-\tau}}, X_i) \) adjacent in \( C(G) \) with \( X_{i_{m-\tau}} < X_i \) do
4: if the middle mark is empty then continue with next pair
5: if \((m = -1 \text{ and } i \neq j) \text{ or } (m \geq 0 \text{ and } \tau \neq m \text{ or } i = j)\) then continue with next pair
6: \( S_{\text{def}}^1 = \text{pa}(\{X_{i_{m-\tau}}, X_i\}, C(G)) \)
7: \( S_{\text{def}}^2 = \text{nodes that have ever been in } \text{pa}(\{X_{i_{m-\tau}}, X_i\}, C(G)) \) since re-initialization
8: \( S_{\text{search}}^1 = \text{napds}_{t_i}(X_{i_{m-\tau}}, X_i) \setminus (S_{\text{def}}^1 \cup S_{\text{def}}^2), \text{ordered according to } I_{\min}(X_i, \cdot) \)
9: \( S_{\text{search}}^2 = \text{napds}_{t_i}(X_{i_{m-\tau}}, X_i) \setminus (S_{\text{def}}^1 \cup S_{\text{def}}^2), \text{ordered according to } I_{\min}(X_{i_{m-\tau}}, \cdot) \)
10: if \(|S_{\text{search}}^1| < p \text{ or } \tau = 0 \text{ and } |S_{\text{search}}^2| < p\) then
11: Update middle mark with \( \cdot \) according to Lemma [S8] continue with next pair
12: for all subsets \( S \subseteq S_{\text{search}}^1 \) with \(|S| = p\) do
13: \( S_{\text{def}} = S_{\text{def}}^1 \cup [S_{\text{def}}^2 \cap \text{napds}_{t_i}(X_{i_{m-\tau}}, X_i, C(G))] \)
14: \((p\text{-value, } I) = \text{CI}(X_{i_{m-\tau}}, X_i, S \cup S_{\text{def}})\)
15: \( I_{\min}(X_{i_{m-\tau}}, X_i) = \min(\{I, I_{\min}(X_{i_{m-\tau}}, X_i)\}) \)
16: if \( p\text{-value} > \alpha \) then
17: mark edge for removal, add \( S \cup S_{\text{def}} \) to \( \text{SepSet}(X_{i_{m-\tau}}, X_i) \)
18: break innermost for-loop
19: if \( \tau = 0 \) then
20: run lines 12 - 18 with \( S_{\text{search}}^2 \) replacing \( S_{\text{search}}^1 \), and \( X_{i_{m-\tau}} \) and \( X_i \) swapped
21: remove all edges that are marked for removal from \( C(G) \)
22: if any edge has been removed in line 21 then
23: run Alg. [S4] using the same rules as in line 22 of Alg. [S2]
24: let \( p = 0 \)
25: else increase \( p \) to \( p + 1 \)
26: until all middle marks in \( C(G) \) are empty
27: run Alg. [S4] using the same rules as in line 22 of Alg. [S2]
28: return \( C(G) \), \( I_{\min}(\cdot, \cdot) \), \( \text{SepSet}(\cdot, \cdot) \)

Algorithm S4 Orientation phase

Require: LPCMCI-PAG \( C(G) \), ordered list of rules \( r \), memory of minimal test statistic values \( I_{\min}(\cdot, \cdot) \), memory of separating sets \( \text{SepSet}(\cdot, \cdot) \), time series dataset \( X = \{X_1, \ldots, X_N\} \), maximal considered time lag \( \tau_{\max} \), significance level \( \alpha \), CI test \( \text{CI}(X, Y, S) \)

1: \( i = 0 \)
2: repeat
3: apply the \( i \)-th rule in \( r \) to \( C(G) \), do not modify \( C(G) \) yet
4: if the rule proposes any modification then
5: for all edges marked for orientation do
6: resolve conflicts among the proposed orientations
7: apply the conflict resolved orientations \( C(G) \)
8: for all edges marked for removal do
9: remove the edge from \( C(G) \)
10: make the corresponding separating set weakly minimal
11: let \( i = 0 \)
12: else increase \( i \) to \( i + 1 \)
13: until \( i \geq \text{len}(r) \)
14: return \( C(G) \), \( I_{\min}(\cdot, \cdot) \), \( \text{SepSet}(\cdot, \cdot) \)
As explained in Sec. S5, Algorithms S2 and S3 respectively perform test of CI given subsets of A weak minimality (whereas this restriction is not necessary weakly minimal is made weakly minimal by successively removing single elements that are not known ancestors of X⁻ᵢ.runners and X⁻ᵢ until the resulting set is no separating set anymore. In particular, there is no need to search through all subsets of the original separating set. The validity of this procedure owes to the equivalence of weak minimality and weak minimality of the second type, see Definition S6 and part 3.) of Lemma S7 below. The algorithm also tests for potential conflicts among the proposed orientations and, if present, resolves them by putting the conflict mark ‘x’. Most rules require to know whether certain nodes are or are not in certain separating sets. Queries of the second type (Is node B not in the separating set of nodes A and C? ) are answered by a modified version of the majority rule proposed in [Colombo and Maathuis, 2014]. Our modification consists of i) searching for separating sets not in the adjacencies of A and C but rather in the relevant apdsᵢ sets and ii) including also those separating sets that were found by Algs. S2 and S3 in the majority vote. The second part of this modification is necessary to guarantee completeness (FCI with the unmodified majority rule is not complete, see Sec. S9 for an example). The modification does not introduce order-independence since i) the sets S_search, S¹_search, and S²_search are ordered by means of Tⁱ⁽ᵐ⁾(·, ·) and since ii) line 13 of Alg. S2 and line 17 of Alg. S3 instruct to add S ∪ Sₐₑₙ to SepSet(X⁻ᵢ₋₉, X⁻ᵢ) rather than saying write to. Point ii) is relevant for contemporaneous links: if in the same iteration of Alg. S2 (Alg. S3) a pair of variables is found to be conditionally independent given subsets of both apdsᵢ(Xᵢ, Xᵢ₊₁, C(G)) and apdsᵢ(Xᵢ, Xᵢ₊₁, C(G)) (both apdsᵢ(Xᵢ, Xᵢ₊₁, C(G)) and napdsᵢ(Xᵢ, Xᵢ₊₁, C(G))), both separating sets are remembered. The search for separating sets involves the same default conditioning as in Alg. S2. For queries of the first type (Is node B in the separating set of nodes A and C?) we distinguish two cases. If B is adjacent to both A and C and the middle mark of both edges is empty, then the query is answered in the same way as queries of the first type. Otherwise, the query is answered solely based on the separating sets found by Algs. S2 and S3. Alternatively, one might also in this second case perform a majority-type search of additional separating sets, albeit restricted to separating sets of minimal cardinality due to the requirement of weak minimality (whereas this restriction is not necessary when A and B as well as C and B are connected by edges with empty middle marks). We do not claim optimality of these choices.

**S6 Definition and relevance apdsᵢ and napdsᵢ sets**

As explained in Sec. S5, Algorithms S2 and S3 respectively perform test of CI given subsets of apdsᵢ sets and napdsᵢ sets. These are defined and motivated here.

In words apdsᵢ(Xᵢ, Xᵢ₋ᵢ₋⁹, C(G)) is the set of all non-future adjacencies of Xᵢ that have not already been identified as non-ancestors of Xᵢ, formally:

**Definition S4 (apdsᵢ sets).** The set apdsᵢ(Xᵢ, Xᵢ₋ᵢ₋⁹, C(G)) is the set of all Xᵢ₋ᵢ₋⁹, other than Xᵢ₋ᵢ, that have not already been identified as non-ancestors of Xᵢ, formally:

**Definition S5 (napdsᵢ sets).** 1) The set napdsᵢ(Xᵢ, Xᵢ₋ᵢ₋⁹, C(G)) is the union of napdsᵢ¹(Xᵢ, Xᵢ₋ᵢ₋⁹, C(G)) and napdsᵢ²(Xᵢ, Xᵢ₋ᵢ₋⁹, C(G)). 2) The set napdsᵢ¹(Xᵢ, Xᵢ₋ᵢ₋⁹, C(G)) is apdsᵢ(Xᵢ, Xᵢ₋ᵢ₋⁹, C(G)) without all variables Xᵢ₋ᵢ₋⁹ that are connected to Xᵢ by an edge with tail at Xᵢ₋ᵢ₋⁹. 3) The set napdsᵢ²(Xᵢ, Xᵢ₋ᵢ₋⁹, C(G)) is the set of all variables Xᵢ₋ᵢ₋⁹ that are connected to Xᵢ by a path p with the following properties: i) on p there is no tail at any node other than Xᵢ₋ᵢ₋⁹, ii) the middle node of every unshielded triple on p is a collider on p, iii) p does not contain Xᵢ₋ᵢ₋⁹, iv) the node Xᵢ₋ᵢ₋⁹ adjacent to Xᵢ is not connected to Xᵢ₋ᵢ by an edge with head at Xᵢ₋ᵢ₋⁹, and is not after Xᵢ₋ᵢ₋⁹, v) all nodes on p other than Xᵢ and Xᵢ₋ᵢ₋⁹ are not connected to Xᵢ or Xᵢ₋ᵢ by an edge with tail at Xᵢ or Xᵢ₋ᵢ, are not at the same time connected to both Xᵢ and Xᵢ₋ᵢ by edges with a head at themselves, and are not after both Xᵢ and Xᵢ₋ᵢ.
The use of the apds$_i$ and napds$_i$ sets in Algorithms S2 and S3 is due to the following result:

**Lemma S3** (Relevance of apds$_i$ and napds$_i$ sets). Let $A$ and $B$ be such that $A \notin \text{adj}(B, \mathcal{M}(\mathcal{G}))$.

1. If $A \in \text{an}(B, \mathcal{G})$ then apds$_i(B, A, \mathcal{C}(\mathcal{G})) \supseteq \text{D-Sep}(B, A, \mathcal{M}(\mathcal{G}))$.
2. If $B \notin \text{an}(A, \mathcal{G})$, $A \notin \text{an}(B, \mathcal{G})$ and rule R0'a has been exhaustively applied to $\mathcal{C}(\mathcal{G})$ then napds$_i(B, A, \mathcal{C}(\mathcal{G})) \supseteq \text{D-Sep}(B, A, \mathcal{M}(\mathcal{G}))$.

This remains true when Definition S5 is strengthened in the following way: Whenever the definition demands that there be no edge between $X_{i-t}^m$ (or $X_i^l$) and some node $X_{m-t}^m$ with head at $X_{m-t}^m$, add the requirement that there be a potentially directed path from $X_{m-t}^m$ to $X_{i-t}^m$ (or $X_i^l$).

## S7 Proofs

**Theorem 1** (LPCMCI effect size). Let $X_{i-t} \rightarrow X_i$ be a link ($\rightarrow$ or $\leftrightarrow$) in $\mathcal{M}(\mathcal{G})$. Denote the union of their parents without $X_i^l$ and $X_{i-t}$ themselves by $\mathcal{P} = \text{pa}((X_{i-t}, X_i), \mathcal{M}(\mathcal{G})) \setminus \{(X_{i-t}, X_i)\}$ and the remaining variables by $\mathbf{X}^* = \mathbf{X} \setminus \mathcal{P}$. Let $\mathbf{S} = \arg \min_{S \subseteq \mathbf{X}^* \setminus \{(X_{i-t}, X_i)\}} I(X_{i-t}^l; X_i^l | S, \mathcal{P})$ be the set of sets that define LPCMCI’s effect size. If there is $\mathbf{S}^* \in \mathbf{S}$ and a proper subset $Q \subset \mathcal{P}$ such that $\mathbf{S}^* \subseteq \text{adj}(X_{i-t}, \mathcal{M}(\mathcal{G})) \setminus \mathbf{P}$ or $\mathbf{S}^* \subseteq \text{adj}(X_i^l, \mathcal{M}(\mathcal{G})) \setminus \mathbf{P}$ and $I(X_{i-t}^l; X_i^l | \mathcal{P} \cup \mathbf{Q}, \mathbf{S}^*, \mathbf{Q}) < 0$, then

\[
\min_{\mathbf{S} \subseteq \mathbf{X}^* \setminus \{(X_{i-t}, X_i)\}} I(X_{i-t}^l; X_i^l | \mathbf{S}, \mathbf{P}) > \min_{\mathbf{S} \subseteq \mathbf{X}^* \setminus \{(X_{i-t}, X_i)\}} I(X_{i-t}^l; X_i^l | \mathbf{S}). \tag{S1}
\]

If the assumptions are not fulfilled, then (trivially) "$\geq" holds in (S1).

**Proof of Theorem 1** We start the proof of eq. (S1) by splitting up the set $\mathbf{X}$ that occurs on its right hand side as follows:

\[
\min_{\mathbf{S} \subseteq \mathbf{X} \setminus \{(X_{i-t}, X_i)\}} I(X_{i-t}^l; X_i^l | \mathbf{S}, \mathbf{P}) > \min_{\mathbf{S} \subseteq \mathbf{X}} I(X_{i-t}^l; X_i^l | \mathbf{S}) \tag{S2}
\]

\[
\Rightarrow \quad \min_{\mathbf{S} \subseteq \mathbf{X} \setminus \{(X_{i-t}, X_i)\}} I(X_{i-t}^l; X_i^l | \mathbf{S}, \mathbf{P}) > \min_{\mathbf{S} \subseteq \mathbf{X} \setminus \{(X_{i-t}, X_i)\}} \min_{\mathbf{Q} \subseteq \mathbf{P}} I(X_{i-t}^l; X_i^l | \mathbf{S}, \mathbf{Q}) \tag{S3}
\]

Note that for $\mathbf{Q} = \mathbf{P}$ the right hand side equals the left hand side. Therefore, eq. (S3) becomes trivially true when "$>$" is replaced by "$\geq"", but as it stands with "$>$" it is equivalent to

\[
\min_{\mathbf{S} \subseteq \mathbf{X} \setminus \{(X_{i-t}, X_i)\}} I(X_{i-t}^l; X_i^l | \mathbf{S}, \mathbf{P}) > \min_{\mathbf{S} \subseteq \mathbf{X} \setminus \{(X_{i-t}, X_i)\}} \min_{\mathbf{Q} \subseteq \mathbf{P}} \min_{\mathbf{Q} \neq \mathbf{P}} I(X_{i-t}^l; X_i^l | \mathbf{S}, \mathbf{Q}), \quad (S4)
\]

where $\mathbf{Q}$ is now restricted to be a proper subset of $\mathbf{P}$. Let, as stated in the theorem, $\mathbf{S}$ be the set of sets that make the left hand side minimal. A sufficient condition for eq. (S4) is then the existence of $\mathbf{S}^* \in \mathbf{S}$ such that

\[
I(X_{i-t}^l; X_i^l | \mathbf{S}^*, \mathbf{P}) > \min_{\mathbf{Q} \subseteq \mathbf{P}, \mathbf{Q} \neq \mathbf{P}} I(X_{i-t}^l; X_i^l | \mathbf{S}^*, \mathbf{Q}). \tag{S5}
\]

Here we have fixed $\mathbf{S} = \mathbf{S}^*$ on the right hand side, taking any other $\mathbf{S} \subseteq \mathbf{X} \setminus \{(X_{i-t}, X_i^l)\}$ in eq. (S4) can only make the right hand side smaller. By subtracting the left hand side of this equation and defining $\mathbf{P}^* = \mathbf{P} \setminus \mathbf{Q}$ we get

\[
\min_{\mathbf{Q} \subseteq \mathbf{P}, \mathbf{Q} \neq \mathbf{P}} \left[ I(X_{i-t}^l; X_i^l | \mathbf{S}^*, \mathbf{Q}) - I(X_{i-t}^l; X_i^l | \mathbf{S}^*, \mathbf{Q}, \mathbf{P}^*) \right] < 0. \tag{S6}
\]

A difference of conditional mutual informations as in this equation defines a trivariate (conditional) interaction information $\mathcal{I}$ [Abramson, 1963; Runge, 2015], such that we can rewrite eq. (S6) as

\[
\min_{\mathbf{Q} \subseteq \mathbf{P}, \mathbf{Q} \neq \mathbf{P}} \mathcal{I}(X_{i-t}^l; X_i^l; \mathbf{P}^* | \mathbf{S}^*, \mathbf{Q}) < 0. \quad (S7)
\]

Contrary to conditional mutual information, the (conditional) interaction information can also attain negative values. This happens when an additional condition, here $\mathbf{P}^*$, increases the conditional mutual information between $X_{i-t}^l$ and $X_i^l$. The second assumption of the theorem states that there is a proper subset $\mathbf{Q} \subset \mathbf{P}$ for which $\mathcal{I}(X_{i-t}^l; X_i^l; \mathbf{P}^* | \mathbf{S}^*, \mathbf{Q}) < 0$. This implies eq. (S7) and hence the main equation (S1).

We now state a Corollary of Theorem 1 which details graphical assumptions that lead to an increase in effect size as required by eq. (S7). Fig. S1 illustrates these graphical criteria.
Corollary S1 (LPCMCI effect size). Let \( X_{i_{-\tau}} \leftrightarrow X_i \) be a link (\( \rightarrow \) or \( \leftrightarrow \)) in \( M(G) \). Denote the union of their parents without \( X_i \) and \( X_{i_{-\tau}} \) themselves by \( P = pa([X_{i_{-\tau}}, X_i], M(G)) \setminus \{X_{i_{-\tau}}, X_i\} \) and the remaining variables by \( X^* = X \setminus P \). Let \( S = \text{arg min}_{S \subseteq X^* \setminus \{X_{i_{-\tau}}, X_i\}} I(X_{i_{-\tau}}; X_i | S, P) \) be the set of sets that define LPCMCI’s effect size. \textbf{Case} \( X_{i_{-\tau}} \rightarrow X_i \): If i) \( pa^*(X_i^*, M(G)) = \mathcal{P} \setminus \{pa(X_{i_{-\tau}}, M(G))\} \) is non-empty (in words: \( X_i \) has parents other than \( X_{i_{-\tau}} \) that are not shared with \( X_i \) and ii) there is \( S^* \in S \) such that \( S^* \subseteq \text{adj}(X_{i_{-\tau}}, M(G)) \setminus \mathcal{P} \) or \( S^* \subseteq \text{adj}(X_i, M(G)) \setminus \mathcal{P} \), and iii) \( X_i \not\in \text{an}(S^*, M(G)) \), and iv) there is no path between \( X_i \) and \( X_{i_{-\tau}} \) and \( pa^*(X_i, M(G)) \) that is active given \( pa(X_{i_{-\tau}}, M(G)) \cup S^* \), and v) faithfulness, then

\[
\min_{S \subseteq X^* \setminus \{X_{i_{-\tau}}, X_i\}} I(X_{i_{-\tau}}; X_i | S, P) > \min_{S \subseteq X^* \setminus \{X_{i_{-\tau}}, X_i\}} I(X_{i_{-\tau}}; X_i | S^*) . \tag{S8}
\]

For the \textbf{case} \( X_{i_{-\tau}} \leftrightarrow X_i \) the same inequality (S8) holds if assumptions i) – iv) hold as stated above or if the assumptions hold with the roles of \( X_i \) and \( X_{i_{-\tau}} \) exchanged. If any of the assumptions is not fulfilled, then (trivially) “\( \geq \)” holds in (S8).

\textbf{Proof of Corollary [S1]} Note that eq. (S8) and eq. (S7) are the same. All manipulations that have identified eq. (S7) as a sufficient condition for eq. (S1) under the assumptions of Theorem [1] are still valid under the assumptions of the corollary. Therefore, eq. (S7) is what remains to be shown.

Since the interaction information is symmetric in its arguments before the “\( \mid \)”, eq. (S7) can be cast into the equivalent conditions:

\[
\min_{Q \subset P, Q \neq P} I(X_{i_{-\tau}}; X_i | S^*, Q) < 0 \tag{S9}
\]

\[
\Leftrightarrow \min_{Q \subset P, Q \neq P} \left[ I(X_{i_{-\tau}}; X_i | S^*, Q) - I(X_{i_{-\tau}}; X_i | S^*, Q, P^*) \right] < 0 \tag{S10}
\]

\[
\Leftrightarrow \min_{Q \subset P, Q \neq P} \left[ I(X_{i_{-\tau}}; P^* | S^*, Q) - I(X_{i_{-\tau}}; P^* | S^*, Q, X_i) \right] < 0 \tag{S11}
\]

\[
\Leftrightarrow \min_{Q \subset P, Q \neq P} \left[ I(P^*; X_i | S^*, Q) - I(P^*; X_i | S^*, Q, X_{i_{-\tau}}) \right] < 0 . \tag{S12}
\]

First consider the case \( X_{i_{-\tau}} \rightarrow X_i \) in conjunction with eq. (S11). Independent of which \( Q \) minimizes the left hand side of this equation, a sufficient condition for its validity is the existence of a proper
We now construct a path from \( S \) to \( p \). Assume without loss of generality that \( \mathcal{S} \) is such that \( \mathcal{S} \) is an ancestor of \( p \). We choose \( \mathcal{S} \) to be any \( \mathcal{S} \) in \( \mathcal{S} \) such that \( \mathcal{S} \) is an ancestor of \( p \). This makes \( \mathcal{S} \) be \( \mathcal{S} \) if \( \mathcal{S} \) is an ancestor of \( p \).

We choose \( \mathcal{S} = \text{pa}(X_i, M(G)) \) and hence get \( \mathcal{P} = \mathcal{P} \setminus \mathcal{Q} = \text{pa}(X_i, M(G)) \). Since by assumption \( \text{pa}(X_i, M(G)) = \mathcal{P} \) is not empty, \( \mathcal{Q} = \text{pa}(X_i, M(G)) \) is indeed a proper subset of \( \mathcal{P} \). Further, eq. \( \text{S13} \) is true by assumption \( \text{iv} \) and eq. \( \text{S14} \) is true by the assumption of faithfulness together with the fact that the path \( X_i \leftarrow X_j \) is active given \( \mathcal{Q} \setminus \mathcal{S} \). Since both conditions in eq. \( \text{S13} \) and eq. \( \text{S14} \) hold for this valid choice of \( \mathcal{Q} \), eq. \( \text{S13} \) and hence the corollary are proven.

We note that assumption \( \text{iii} \) is needed. Otherwise conditioning on \( \mathcal{S} \) opens the path \( X_i \leftarrow X_j \) since \( X_i \) is an ancestor of a conditioned node, thus assumption \( \text{iv} \) could not be true. Assumption \( \text{ii} \) would be violated by the assumptions connections shown in Fig. \( \text{S1} \) if \( \text{pa}(X_i, M(G)) \) is empty or another assumption does not hold, the inequality \( \text{S1} \) may still hold, but in any case \( \text{ii} \) can be replaced by \( \text{ii} \).

In the case \( X_i \leftarrow X_j \) we can either utilize eq. \( \text{S11} \) or eq. \( \text{S12} \), depending on whether \( X_i \) or \( X_j \) (or both) contain non-empty non-shared parents for which eq. \( \text{S13} \) and eq. \( \text{S14} \) or the equivalent assumptions with \( X_i \) and \( X_j \) exchanged hold. Lastly, the case \( X_i \leftarrow X_j \) is covered by simply exchanging \( X_i \) and \( X_j \).

Lemma \( \text{S4} \) (Inclusion of ancestors in separating sets). Let \( A \) and \( B \) be \( m \)-separated given \( S \), and let \( \mathcal{S}_{\text{def}} \subseteq \text{an}(\{A, B\}, M(G)) \setminus \{A, B\} \) be arbitrary. Then, \( A \) and \( B \) are also \( m \)-separated given \( \mathcal{S}' = S \cup \mathcal{S}_{\text{def}} \).

Proof of Lemma \( \text{S4} \). Assume without loss of generality that \( \mathcal{S}_{\text{def}} \) is non-empty, else the statement is trivial. First, consider the case \( \mathcal{S}_{\text{def}} \subseteq \text{an}(B, M(G)) \) and assume \( \mathcal{S}' \) did not \( m \)-separate \( A \) and \( B \). This requires the existence of a path \( p \) between \( A \) and \( B \) for which \( a1 \) at least one non-collider on \( p \) is in \( S \) or \( a2 \) there is a collider on \( p \) that is not an ancestor of \( S, b \) none of the non-colliders on \( p \) is in \( S' \), and \( c \) all colliders on \( p \) are ancestors of \( S' \). Since \( S \) is a proper subset of \( S', a1 \) conflicts with \( b \). This means \( a2 \) must be true, i.e., there is at least one collider on \( p \) that is an ancestor of \( S', S \) \( \subseteq \text{an}(B, M(G)) \) and hence of \( B \). Among all those collider, let \( C \) be the one closest to \( A \) on \( p \). According to \( b \) the sub-path \( \text{p}_{\text{AC}} \) of \( p \) from \( A \) to \( C \) is then active given \( \mathcal{S} \) by construction. Since \( C \) is an ancestor of \( B \) there is at least one directed path \( \text{p}_{\text{CB}} \) from \( C \) to \( B \). By definition of \( C \) the path \( \text{p}_{\text{CB}} \) does not cross any node in \( S \). Thus, \( \text{p}_{\text{CB}} \) is active given \( S \).

We now construct a path from \( A \) to \( B \) that is active given \( S \), thereby reaching a contradiction. To this end, let \( D \) be the node closest to \( A \) on \( \text{p}_{\text{AC}} \) that is also on \( \text{p}_{\text{CB}} \) (such \( D \) always exists, because \( C \) is on both paths). Consider then the subpath \( \text{p}_{\text{AD}} \) of \( \text{p}_{\text{AC}} \) from \( A \) to \( D \), and the subpath \( \text{p}_{\text{DB}} \) on \( \text{p}_{\text{CB}} \) from \( D \) to \( B \). Since \( \text{p}_{\text{AC}} \) and \( \text{p}_{\text{CB}} \) are active given \( S \), also \( \text{p}_{\text{AD}} \) and \( \text{p}_{\text{DB}} \) are active given \( S \). By definition of \( D \) the concatenation of \( \text{p}_{\text{AD}} \) and \( \text{p}_{\text{DB}} \) at their common end \( D \) gives a path \( \text{p}_{\text{AB}} \) from \( A \) to \( B \). Since \( D \) is a non-collider on \( \text{p}_{\text{AB}} \) (because \( \text{p}_{\text{DB}} \) is out of \( D \)) and \( D \) is not in \( S \) (because else \( C \) would be an ancestor of \( S \)), \( \text{p}_{\text{AB}} \) is active given \( S \). Contradiction.

Second, since the Lemma does not make any distinction between \( A \) and \( B \), it is also true in case \( \mathcal{S}_{\text{def}} \subseteq \text{an}(A, M(G)) \). Third, write \( S = S_A \cup S_B \) with \( S_A = S \cap \text{an}(A, M(G)) \) and \( S_B = S \setminus S_A \subseteq \text{an}(B, M(G)) \). The statement then follows from applying the already proven special cases twice.

Lemma \( \text{S5} \) (Exclusion of non-ancestors and future from separating sets). Let \( A \) and \( B \) be \( m \)-separated given \( S \), and let \( \mathcal{U} \) be such that \( \mathcal{U} \setminus \text{an}(\{A, B\}, S \setminus \mathcal{U}, M(G)) = \emptyset \). Then, \( A \) and \( B \) are also \( m \)-separated given \( S' = S \setminus \mathcal{U} \). Two important special cases are: 1. \( \mathcal{U} = \emptyset \) \( \mathcal{U} \), which allows to restrict separating sets to ancestors. 2. \( \mathcal{U} = \{\text{nodes that are in the future of both } A \text{ and } B\} \), which allows to restrict separating sets to the present and past of the later variable.

Proof of Lemma \( \text{S5} \). Assume without loss of generality that \( \mathcal{U} \) is non-empty, else the statement is trivial. Assume \( \mathcal{U} \) did not \( m \)-separate \( A \) and \( B \). This requires the existence of a path \( p \) between \( A \) and \( B \) for which \( a1 \) at least one non-collider on \( p \) is in \( \mathcal{S} \) or \( a2 \) there is a collider on \( p \) that is not an ancestor of \( S, b \) none of the non-colliders on \( p \) is in \( \mathcal{S}' \), and \( c \) all colliders on \( p \) are ancestors of \( \mathcal{S}' \). Since \( \mathcal{S}' \) is a proper subset of \( \mathcal{S}, a2 \) conflicts with \( c \). This means \( a2 \) must be true, i.e.,
there is a non-collider \( D \) on \( p \) in \( S \setminus S' = S \cap U \). In particular, \( D \) is in \( U \). All nodes on \( p \) are ancestors of \( A \) or \( B \) or of a collider on \( p \). If \( D \) is an ancestor of a collider on \( p \), then by \( c \) it is also an ancestor of \( S' = S \setminus U \). This shows that \( D \) is also in \( an(\{A, B, S \setminus U\}, \mathcal{M}(\mathcal{G})) \). Since \( U \cap an(\{A, B, S \setminus U\}, \mathcal{M}(\mathcal{G})) = \emptyset \), this is a contradiction.

**Special case 1.** For \( \mathcal{U} = S \setminus an(\{A, B\}, \mathcal{M}(\mathcal{G})) \) we have \( S' = S \cap an(\{A, B\}, \mathcal{M}(\mathcal{G})) \) and \( an(\{A, B, S \setminus U\}, \mathcal{M}(\mathcal{G})) = an(\{A, B\}, \mathcal{M}(\mathcal{G})) \). Hence, the condition is fulfilled. **Special case 2.** For \( \mathcal{U} = \{ \text{all nodes that are in the future of both } A \text{ and } B \} \) we have \( an(\{A, B, S \setminus U\}, \mathcal{M}(\mathcal{G})) \subseteq \{ \text{all nodes that are not after both } A \text{ and } B \} \). Hence, the condition is fulfilled.

Note that if \( \mathcal{U} \) fulfills the above condition, a proper subset \( \mathcal{U}' \) of \( \mathcal{U} \) does not necessarily fulfill the condition as well. Consider the example \( A \rightarrow C \leftarrow D \rightarrow B \). Here \( S = \{C, D\} \) m-separates \( A \) and \( B \), and \( \mathcal{U} = S \) fulfills the condition. However, \( \mathcal{U}' = \{C\} \) does not. This is why we need to require \( \mathcal{U} \cap an(\{A, B, S \setminus U\}, \mathcal{M}(\mathcal{G})) = \emptyset \) and not just \( \mathcal{U} = an(\{A, B\}, \mathcal{M}(\mathcal{G})) = \emptyset \).

**Lemma S6** (Some properties of D-Sep sets). Consider two distinct nodes \( A, B \in \mathcal{M}(\mathcal{G}) \). Let \( V \in D-Sep(B, A, \mathcal{M}(\mathcal{G})) \) and \( p_{V} \) be as in Definition S2, and denote with \( C \neq B \) the node on \( p_{V} \) that is closest to \( B \). 1.) If \( A \notin adj(B, \mathcal{M}(\mathcal{G})) \), then \( p_{V} \) does not contain \( A \). 2.) If \( B \notin an(A, \mathcal{G}) \) and \( p_{V} \) contains two nodes only, then \( C \) is a parent or spouse of \( B \). 3.) If \( B \notin an(A, \mathcal{G}) \) and \( p_{V} \) contains more than two nodes, then \( C \) is a spouse of \( B \) and ancestor of \( A \). 4.) If \( A \in an(B, \mathcal{G}) \), then \( D-Sep(B, A, \mathcal{M}(\mathcal{G})) = pa(B, \mathcal{M}(\mathcal{G})) \).

**Proof of Lemma S6.** 1.) Assume \( p_{V} \) did contain \( A \). The subpath of \( p_{V} \) from \( B \) to \( A \) is then an inducing path between \( B \) and \( A \). Since \( A \) and \( B \) are not adjacent, this violates maximality of the MAG \( M \). 2.) By construction \( V = C \) is adjacent to \( B \). Assume \( C \) was a child of \( B \). Since \( C \) must be an ancestor of \( A \) or \( B \), \( C \) must be an ancestor of \( A \). Then \( B \) is an ancestor of \( A \), contrary to the assumption. 3.) According to the second part \( C \) is a parent or spouse of \( B \). If \( C \) was a parent of \( B \), \( C \) would be a non-collider on \( p_{V} \). This contradicts the definition of \( p_{V} \), hence \( C \) is a spouse of \( B \). Moreover, since \( C \) is an ancestor of \( A \) or \( B \), \( C \) is an ancestor of \( A \). 4.) The inclusion \( D-Sep(B, A, \mathcal{M}(\mathcal{G})) \supseteq pa(B, \mathcal{M}(\mathcal{G})) \) follows since \( V \) is a parent of \( B \) then \( V \rightarrow B \) is a path as required by the definition. We now show the opposite inclusion \( D-Sep(B, A, \mathcal{M}(\mathcal{G})) \subseteq pa(B, \mathcal{M}(\mathcal{G})) \) by showing that \( V \in pa(B, \mathcal{M}(\mathcal{G})) \). Case 1: \( p_{V} \) has two nodes only. By the second part of this Lemma \( V \) is a parent or spouse of \( B \). Assume it was a spouse. Then \( V \) must be an ancestor of \( A \), which with \( A \in an(B, \mathcal{G}) \) gives \( C \in an(B, \mathcal{G}) \). But then \( C \) cannot be a spouse of \( B \). Case 2: \( p_{V} \) has more than three nodes. By the third part of this Lemma we then get that \( C \) is an ancestor of \( A \), which again leads to the contradiction \( C \in an(B, \mathcal{G}) \). □

**Proof of Lemma S3.** 1.) \( A \in an(B, \mathcal{G}) \) gives \( D-Sep(B, A, \mathcal{M}(\mathcal{G})) = pa(B, \mathcal{M}(\mathcal{G})) \) by part 4.) of Lemma S6. Consider \( C \in pa(B, \mathcal{M}(\mathcal{G})) \). Then, \( C \) is adjacent to \( B \) in \( \mathcal{G}(\mathcal{M}) \) with a link that does not have a head at \( C \). Moreover, \( C \) cannot be after \( B \). Since \( A \) and \( B \) are not adjacent, \( C \) cannot be \( B \). Hence \( C \) in \( apds_{1}(B, A, \mathcal{G}(\mathcal{M})) \). 2.) Consider \( V \in D-Sep(B, A, \mathcal{M}(\mathcal{G})) \) and let the path \( p_{V} \) be as in Definition S2. Case 1: \( V \) is a parent of \( B \) in \( \mathcal{G}(\mathcal{M}) \). Then, as the proof of the first part of this Lemma shows \( V \in apds_{1}(B, A, \mathcal{G}(\mathcal{M})) \). Now assume \( V \) was a child of \( A \) in \( \mathcal{G}(\mathcal{M}) \). Then \( A \in an(B, \mathcal{G}) \), contradicting the assumption. Hence \( V \in apds_{2}^{1}(B, A, \mathcal{G}(\mathcal{M})) \). Case 2: \( V \) is not a parent of \( B \) in \( \mathcal{G}(\mathcal{M}) \). We now show that \( p_{V} \) is a path \( p \) as required in 3.) of Definition S5, and hence \( V \in apds_{2}^{1}(B, A, \mathcal{G}(\mathcal{M})) \). Let \( C \) be the node on \( p_{V} \) that is closest to \( B \), which by 2.) and 3.) of Lemma S6 is a spouse of \( B \). i) is true since all non end-point nodes on \( p_{V} \) are colliders on \( p \), together with the fact that \( C \) is a spouse of \( B \). ii) is true for the same reason as i) together with the fact that rule R0/a has been exhaustively applied, which guarantees that if an unshielded triple is a collider then it will be oriented as a collider. iii) is true by 1.) of Lemma S6. iv) is true since \( C \) is an ancestor of \( A \) by 3.) of Lemma S6. The second and third part of v) are true since all nodes on \( p_{V} \) are ancestors of \( A \) or \( B \). For the first part of v) observe that if \( V \) is a descendant of \( A \) (or \( B \)) in \( \mathcal{G}(\mathcal{M}) \), then since \( V \) is an ancestor of \( A \) or \( B \) we would get \( A \in an(B, \mathcal{G}) \) (or \( B \in an(A, \mathcal{G}) \)), a contradiction.

**Definition S6** (Weakly minimal separating sets of the second type). In MAG \( \mathcal{M}(\mathcal{G}) \) let \( A \) and \( B \) be m-separated by \( S \). The set \( S \) is a weakly minimal separating set of \( A \) and \( B \) of the second type if i) there is a decomposition \( S = S_{1} \cup S_{2} \) with \( S_{1} \subseteq an(\{A, B\}, \mathcal{M}(\mathcal{G})) \) such that ii) if there is \( S \in S_{2} \) such that \( S' = S \setminus S \) is a separating set of \( A \) and \( B \) then \( S \in an(\{A, B\}, \mathcal{M}(\mathcal{G})) \). The pair \((S_{1}, S_{2})\) is called a weakly minimal decomposition of \( S \) of the second type.

**Lemma S7** (Selected properties of weakly minimal separating sets). 1.) \( S \) is a weakly minimal separating set of the second type if and only if its canonical decomposition \((T_{1}, T_{2})\) defined by...
\( T_1 = S \cap an(\{A, B\}, M(\mathcal{G})) \) and \( T_2 = S \setminus T_1 \) is a weakly minimal decomposition of \( S \) of the second type. 2.) If \( S \) is a weakly minimal separating set of \( A \) and \( B \) of the second type then \( \mathcal{S} \subseteq an(\{A, B\}, M(\mathcal{G})) \subseteq an(\{A, B\}, \mathcal{G}) \). 3.) \( S \) is a weakly minimal separating set of the second type if and only if it is a weakly minimal separating set. 4.) \( S \) is a weakly minimal separating set of \( A \) and \( B \) if and only if it is a separating set of \( A \) and \( B \) and \( S \subseteq an(\{A, B\}, M(\mathcal{G})) \subseteq an(\{A, B\}, \mathcal{G}) \). 5.) If \( S \) is a non-weakly minimal separating set of \( A \) and \( B \) then there is a proper subset \( S' \) of \( S \) that is a weakly minimal separating set of \( A \) and \( B \).

**Proof of Lemma [S7]** 1.) if: The existence of a weakly minimal decomposition of the second type implies weak minimality of the second type. 1.) only if: By assumption there is some weakly minimal decomposition \( (S_1, S_2) \) of the second type. By definition of the canonical decomposition and by condition \( i \) in Definition [S6] the inclusions \( S_1 \subseteq T_1 \) and hence \( S_2 \subseteq T_2 \) hold. Assume the canonical decomposition were not a weakly minimal decomposition of \( S \) of the second type. Then there is some \( S \in T_2 \) such that \( S' = S \setminus S \) is a separating set. Since \( S_2 \subseteq T_2 \) then also \( S \in S_2 \), contradicting the assumption that \( (S_1, S_2) \) is a weakly minimal decomposition of the second type. 2.) Since \( S \) is weakly minimal of the second type, its canonical decomposition \( (T_1, T_2) \) is a weakly minimal decomposition of \( S \) of the second type. We now show that \( T_2 \) must be empty. Assume it was not and let \( C_1, \ldots, C_n \) be its elements. Since by construction \( C_1 \notin an(\{A, B\}, M(\mathcal{G})) \) and since \( (T_1, T_2) \) is weak minimal decomposition of the second type, \( A \) and \( B \) are not \( m \)-separated by \( S' = S \setminus C_1 \). This means there is a path \( p \) that is active given \( S' \) and blocked given \( S \). Hence, \( C_1 \) must be a non-collar on \( p \). Together with \( C_1 \notin an(\{A, B\}, M(\mathcal{G})) \) this shows that \( C_1 \) is an ancestor of some collider \( D_1 \) on \( p \), which itself is an ancestor of \( S' \) (else \( p \) would not be active given \( S' \)). Hence, \( C_1 \) is an ancestor \( S' \). Since \( C_1 \notin an(\{A, B\}, M(\mathcal{G})) \) and \( T_1 \subseteq an(\{A, B\}, M(\mathcal{G})) \), \( C_1 \) is an ancestor of \( \{C_2, \ldots, C_n\} \). If \( n = 1 \), this is a contradiction already. If \( n > 1 \) we may without loss of generality assume that \( C_1 \) is an ancestor of \( C_2 \). Hence, \( C_2 \) is not an ancestor of \( C_1 \). By applying the same argument to \( C_2 \), we conclude that \( C_2 \) is an ancestor of \( \{C_3, \ldots, C_n\} \). Repeat this until reaching a contradiction. This shows \( T_2 = \emptyset \) and hence \( S \subseteq an(\{A, B\}, M(\mathcal{G})) \subseteq an(\{A, B\}, \mathcal{G}) \). 3.) if: Condition \( ii \) in Definition [S4] is clearly stronger than \( ii \) in Definition [S6]. 3.) only if: Let \( S \) be a weakly minimal separating set of the second type, for which by part 2.) of this Lemma \( S \subseteq an(\{A, B\}, M(\mathcal{G})) \). Therefore, \( (S, \emptyset) \) is a weakly minimal decomposition of \( S \), showing that \( S \) is weakly minimal. 4.) if: \( (S, \emptyset) \) is a weakly minimal decomposition 4.) only if: This follows from parts 2.) and 3.) of this Lemma. 5.) According to (the first special case of) Lemma [S5] \( S' = S \cap an(\{A, B\}, M(\mathcal{G})) \) is a separating set. This \( S' \) is weakly minimal according to part 4.) of this Lemma. □

**Lemma 1** (Ancestor-parent-rule). In LPCMCI-PAG \( C(\mathcal{G}) \) one may replace 1.) \( A \rightarrow B \) by \( A \rightarrow B \), 2.) \( A \leftrightarrow B \) for \( A > B \) by \( A \rightarrow B \), and 3.) \( A \leftrightarrow B \) for \( A < B \) by \( A \rightarrow B \).

**Proof of Lemma [S1] 2.)** By the fourth point in Definition [S3] \( A \notin an(B, \mathcal{G}) \) or there is no \( S \subseteq pa(B, M(\mathcal{G})) \) that \( m \)-separates \( A \) and \( B \) in \( M(\mathcal{G}) \). The first option contradicts \( A \rightarrow B \), so the second option must be true. Since \( A \in an(B, \mathcal{G}) \) gives \( D-Sep(B, A, M(\mathcal{G})) = pa(B, M(\mathcal{G})) \) according to part 4.) of Lemma [S6] Proposition [S7] then implies that \( A \) and \( B \) are not \( m \)-separated by any set. 3.) Equivalent proof. 1.) Recall that if \( A \rightarrow B \) in \( C(\mathcal{G}) \), then both \( A \leftrightarrow B \) and \( A \leftrightarrow B \) would be correct. The statement then follows since either 2.) or 3.) of this Lemma applies. □

**Lemma 2** (Strong unshielded triple rule). Let \( A \leftrightarrow B \leftrightarrow C \) be an unshielded triple in LPCMCI-PAG \( C(\mathcal{G}) \) and \( S_{AC} \) the separating set of \( A \) and \( C \). 1.) If \( i \) \( B \in S_{AC} \) and \( ii \) \( S_{AC} \) is weakly minimal, then \( B \in an(\{A, C\}, \mathcal{G}) \). 2.) Let \( T_{AB} \subseteq an(\{A, B\}, M(\mathcal{G})) \) and \( T_{CB} \subseteq an(\{C, B\}, M(\mathcal{G})) \) be arbitrary. If \( i \) \( B \notin S_{AC} \), \( ii \) \( A \) and \( B \) are not \( m \)-separated by \( S_{AC} \cup T_{AB} \setminus \{A, B\} \), \( iii \) \( C \) and \( B \) are not \( m \)-separated by \( S_{AC} \cup T_{CB} \setminus \{C, B\} \), then \( B \notin an(\{A, C\}, \mathcal{G}) \). The conditioning sets in \( ii \) and \( iii \) may be intersected with the past and present of the later variable.

**Proof of Lemma [S2] 1.)** This follows immediately from part 4.) of Lemma [S7] 2.) By the contraposition of Lemma [S4] (condition \( ii \)) implies that \( A \) and \( B \) are not \( m \)-separated by \( S_{AC} \), and similarly \( iii \) implies the same for \( C \) and \( B \). The additional claims made in the last sentence of the Lemma follow by the contraposition of Lemma [S5] The statement then follows from Lemma 3.1 in [Colombo et al., 2012]. Although there minimality of \( S_{AC} \) is stated as an additional assumption, the proof given in the supplement to [Colombo et al., 2012] does not use this assumption. □

**Proof of the orientation rules given in subsection [S4]** Whenever neither a rule consequent nor the hypothetical manipulations involved in its proof require that a certain edge mark be oriented as head or tail, the rule also applies when that edge mark is the conflict mark ‘\( \cdot \)’. This explains the use of ‘\( \leftrightarrow \)’ vs. ‘\( \rightarrow \)’ marks in the rule antecedents. We repeat that if \( X \leftrightarrow Y \rightarrow Z \) is an unshielded triple and a rule
requires \( Y \in \mathcal{S}_{XZ} \) with \( \mathcal{S}_{XZ} \) weakly minimal, the requirement of weak minimality may be dropped if \( X \rightarrow Y \rightarrow Z \). This is true since when \( X \rightarrow Y \rightarrow Z \) we can conclude \( Y \in \text{an}(\{X, Z\}, \mathcal{G}) \) from \( Y \in \mathcal{S}_{XZ} \) even if \( \mathcal{S}_{XZ} \) is not weakly minimal.

**R0a:** This follows from the second part Lemma 3. Requirement \( iii \) is irrelevant in the case of perfect statistical decisions, it will then never be true given that \( iia \) or \( iib \) and \( iii \) or \( iib \) are true.

**R0b:** Assume \( B \in \text{an}(C, \mathcal{G}) \) were true. By Lemma 1 then \( B \rightarrow C \) in \( \mathcal{C}(\mathcal{G}) \) and hence in \( \mathcal{M}(\mathcal{G}) \). Since one of \( iia \) or \( iib \) is true by assumption, there is a path \( p_{AB} \) from \( A \) to \( B \) that is active given \( \{ A, B \} \). Due to Lemmas 4 and 5 and since \( B \notin \mathcal{S}_{AC}, p_{AB} \) is also active given \( \mathcal{S}_{AC} \). Since then every subpath of \( p_{AB} \) is active given \( \mathcal{S}_{AC} \) and since \( \mathcal{S}_{AC} \) is a separating set of \( A \) and \( C \), \( C \) cannot be on \( p_{AB} \). When appending the edge \( B \rightarrow C \) to \( p_{AB} \) we hence obtain a path \( p_{AC} \). Since \( B \) is a non-collider on \( p_{AC} \) and \( B \notin \mathcal{S}_{AC} \), \( p_{AC} \) is active given \( \mathcal{S}_{AC} \). Contradiction. Hence \( B \notin \text{an}(C, \mathcal{G}) \).

**R0c:** Assume \( B \in \text{an}(C, \mathcal{G}) \) were true. By Lemma 1 then \( B \rightarrow C \) in \( \mathcal{C}(\mathcal{G}) \) and hence in \( \mathcal{M}(\mathcal{G}) \). Moreover \( A \rightarrow B \) or \( A \leftrightarrow B \) or \( A \rightarrow B \) in \( \mathcal{M}(\mathcal{G}) \) by assumption. In either case \( A, B \) and \( C \) form an unshielded triple in \( \mathcal{M}(\mathcal{G}) \) with its middle node \( B \) not being a collider. But then \( B \in \mathcal{S}_{AC} \). Contradiction. Hence \( B \notin \text{an}(C, \mathcal{G}) \).

**R0d:** Since all involved middle marks are empty this is just the standard FCI rule \( R0 \).

**R1’:** From the first part of Lemma 2 we get \( B \in \text{an}(\{A, C\}, \mathcal{G}) \). Due to the head at \( B \) on its edge with \( A \) we know \( B \notin \text{an}(A, \mathcal{G}) \). Hence \( B \notin \text{an}(C, \mathcal{G}) \).

**R2’:** Assume \( C \in \text{an}(A, \mathcal{G}) \) were true. Case 1: \( A \rightarrow B \rightarrow C \). Due to transitivity of ancestry then also \( C \in \text{an}(B, \mathcal{G}) \). This contradicts the head at \( C \) on its edge with \( B \). Case 2: \( A \rightarrow B \rightarrow C \). Then \( B \in \text{an}(A, \mathcal{G}) \), contradicting the head at \( B \) on its link with \( A \). Hence \( C \notin \text{an}(A, \mathcal{G}) \).

**R3’:** Assume \( B \in \text{an}(D, \mathcal{G}) \) were true. By applying the first part of Lemma 2 to the unshielded triple \( A \rightarrow D \rightarrow B \) we deduce that \( D \in \text{an}(\{A, C\}, \mathcal{G}) \). Thus \( B \in \text{an}(\{A, C\}, \mathcal{G}) \), contradicting at least one of the heads at \( B \) in the triple \( A \rightarrow B \rightarrow C \). Hence \( B \notin \text{an}(D, \mathcal{G}) \).

**R4’:** This follows from Lemma 3.2 in [Colombo et al., 2012] together with \( i \) the contrapositions of Lemmas 4 and 5 and \( ii \) that a pair of variables which in \( \mathcal{C}(\mathcal{G}) \) is connected by an edge with empty middle mark then this pair of variables is also adjacent in \( \mathcal{M}(\mathcal{G}) \).

**R8’:** Transitivity of ancestry gives \( A \in \text{an}(C, \mathcal{G}) \), hence also \( C \notin \text{an}(A, \mathcal{G}) \).

**R9’:** Assume \( A_{-1} \notin \text{an}(A_0, \mathcal{G}) \) were true, such that \( A_0 \rightarrow A_{-1} \). By application of the first part of Lemma 2 to the unshielded triple \( A_{-1} \rightarrow A_0 \rightarrow A_1 \) we would then conclude \( A_0 \rightarrow A_1 \). For all unshielded triples \( A_k \rightarrow A_{k+1} \rightarrow A_{k+2} \) on the path from \( A_0 \) to \( A_{-1} \) through \( A_1, \ldots, A_n \) (in this order) we get \( A_{k+2} \rightarrow A_{k+1} \) from \( iia \) or from \( iib \) together with the first part of Lemma 2. This gives \( A_0 \in \text{an}(A_{-1}, \mathcal{G}) \), which contradicts the head at \( A_0 \) on \( A_{-1} \rightarrow A_0 \). Hence \( A_{-1} \notin \text{an}(A_0, \mathcal{G}) \).

**R10’:** Application of the first part of Lemma 2 to the unshielded triple \( B_1 \rightarrow B_2 \rightarrow B_3 \) gives \( A \in \text{an}(\{B_1, C_1\}, \mathcal{G}) \). Say, without loss of generality, \( A \in \text{an}(B_1, \mathcal{G}) \). For all unshielded triples \( B_k \rightarrow B_{k+1} \rightarrow B_{k+2} \) on the path from \( B_1 \) to \( B_3 \), through \( B_2, B_3, \ldots, B_{n-1} \) (in this order) we get \( B_{k+2} \rightarrow B_{k+1} \) from \( iia \) or from \( iib \) together with the first part of Lemma 2. This shows that \( A \in \text{an}(D, \mathcal{G}) \).

**APR:** These are the replacements specified in Lemma 1 which was already proven above.

**MMR:** This follows immediately from the causal meaning of middle marks ‘L’, ‘R’, and ‘!’ given in Definition 3.

**Lemma S8** (Symbolic middle mark update). Middle marks can be updated by the symbolic rules ‘?’ + ‘*’ = ‘*’, ‘*’ + ‘?’ = ‘?’ and ‘L’ + ‘R’ = ‘!’. 

**Proof of Lemma S8** The first rule follows since the middle mark ‘?’ does not make any statement, hence it is consistent with all other middle marks. The second rule follows since the statement made by the empty middle mark ‘’ implies the statements made by all other middle marks. The third rule follows from the definition of the middle mark ‘!’.

**Lemma S9** (Algorithm S2). Assume Algorithm S2 is being passed a LPCMCI-PAG \( \mathcal{C}(\mathcal{G}) \) as well as the assumptions stated in Theorem 2.1. \( \mathcal{C}(\mathcal{G}) \) remains a LPCMCI-PAG at any point of the algorithm. 2.) The algorithm converges.
Proof of Lemma \(S9\). Write \(A = X_{i-1}^i\) and \(B = X_j^j\). 1.) Given faithfulness and perfect statistical decisions, edges are removed if and only if the corresponding nodes are \(m\)-separated by some subset of variables. The for-loop in line 3 considers ordered pairs \((A, B)\) only if \(A < B\) with respect to the adopted total order \(<\). According to Lemma \(S4\), the default conditioning on parents as described by lines 5 and 10 does not destroy any \(m\)-separations. The algorithm therefore updates the edge between \(A\) and \(B\) with middle mark ‘R’ only if \(A\) and \(B\) are not \(m\)-separated by any subset of \(\operatorname{apds}_t(B, A, C(G))\). Since \(pa(B, M(G)) \subseteq \operatorname{apds}_t(B, A, C(G))\) holds, \(A\) and \(B\) are then not \(m\)-separated by any subset of \(pa(B, M(G))\) and the update is correct. Similarly the update with middle mark ‘L’ is correct. Note that the algorithm resets \(p = 0\) once any edge marks have been updated, i.e., once some default conditioning sets may potentially change. Therefore, all separating sets found by the algorithm are weakly minimal. More formally: The default conditioning set \(S_{\text{def}}\) corresponds to \(S_1\) in Definition \(S4\) and \(S\) corresponds to \(S_2\). Whenever \(S_1\) changes, the algorithm restarts with \(|S_2| = p = 0\) and keeps increasing \(p\) by steps of one. If the algorithm finds that some pair of variables is conditionally independent given \(S_{\text{def}} \cup S\), this pair of variables is not conditionally independent given \(S_{\text{def}} \cup S'\) for a proper subset \(S'\) of \(S\). This is because CI given \(S_{\text{def}} \cup S'\) was tested before and rejected, if it would not have been rejected the edge would have been removed already. The statement then follows from correctness of the orientation rules, which is already proven. 2.) If \(A\) and \(B\) are connected by a link with middle mark ‘?’ or ‘L’, the algorithm keeps testing for CI given subsets of \(\operatorname{apds}_t(B, A, C(G))\) until the link has been removed or updated with middle mark ‘R’. Similarly, if \(A\) and \(B\) are connected by a link with middle mark ‘?’ or ‘R’, the algorithm keeps testing for CI given subsets of \(\operatorname{apds}_t(A, B, C(G))\) until the link has been removed or update with middle mark ‘L’. There is no orientation rule that turns a middle mark ‘!’ back into ‘?’ or ‘L’, or ‘R’, and there is no orientation rule that modifies an empty middle mark. With the update rules given in Lemma \(S8\) this shows that all remaining edges will eventually have middle marks ‘!’ or ‘?’ (empty). Then, the algorithm converges. \(\square\)

Lemma \(S10\) (An implication of middle mark ‘!’). Assume \(A \!\implies B\) in LPCMCI-PAG \(C(G)\) but \(A \notin \operatorname{adj}(B, M(G))\). Then: 1.) \(A \notin \operatorname{an}(B, G)\) and \(B \notin \operatorname{an}(A, G)\). 2.) Assume further that \(R0\alpha\) has been exhaustively applied to \(C(G)\). Then, \(A\) and \(B\) are \(m\)-separated by a subset of \(\operatorname{napds}_t(B, A, C(G))\) and by a subset of \(\operatorname{napds}_t(A, B, C(G))\).

Proof of Lemma \(S10\). Without loss of generality we can assume that \(A < B\). 1.) Assume \(A \in \operatorname{an}(B, G)\) were true. Then \(A\) and \(B\) would be \(m\)-separated by some subset of \(\operatorname{D-Sep}(B, A, M(G))\) for which \(\operatorname{D-Sep}(B, A, M(G)) = pa(B, M(G))\) by 4.) of Lemma \(S6\). This contradicts \(A \!\implies B\) and hence \(A \!\leftarrow B\). Similarly \(B \in \operatorname{an}(A, G)\) contradicts \(A \!\leftarrow B\) and hence \(A \!\leftarrow B\). 2.) This follows from the first part together with Lemma \(S5\). \(\square\)

Lemma \(S11\) (Algorithm \(S3\)). Assume Algorithm \(S3\) is being passed a LPCMCI-PAG \(C(G)\). 1.) \(C(G)\) remains a LPCMCI-PAG at any point of the algorithm. 2.) The algorithm converges.

Proof of Lemma \(S11\). Write \(A = X_{i-1}^i\) and \(B = X_j^j\). 1.) An edge between \(A\) and \(B\) is updated with the empty middle mark only if \(A\) and \(B\) are not \(m\)-separated by a subset of \(\operatorname{napds}_t(A, B, C(G))\) or \(\tau = 0\) and \(A\) and \(B\) are not \(m\)-separated by a subset of \(\operatorname{napds}_t(A, B, C(G))\). Note that \(R0\alpha\) is exhaustively applied in line 22 of Alg. \(S2\), as well as in line 23 of Alg. \(S3\). According to Lemma \(S10\) the update is then correct. Apart from this the proof parallels the proof of 1.) of Lemma \(S9\). 1.) If \(A\) and \(B\) are connected by a link with middle mark ‘!’ then the algorithm keeps testing for CI given subsets of \(\operatorname{napds}_t(A, B, C(G))\) and if \(\tau = 0\) also given subsets of \(\operatorname{napds}_t(A, B, C(G))\) until the link has been removed or updated with the empty middle mark. There is no orientation rule that turns a middle mark ‘!’ back into ‘?’ or ‘L’, or ‘R’, and there is no orientation rule that modifies an empty middle mark. With the update rules given in Lemma \(S8\) this shows that all remaining edges will eventually have empty middle marks. Then, the algorithm converges. \(\square\)

Theorem 2 (LPCMCI is sound and complete). Assume that there is a process as in eq. 1 without causal cycles, which generates a distribution \(P\) that is faithful to its time series graph \(G\). Further assume that there are no selection variables, and that we are given perfect statistical decisions about CI in the marginal of \(P\). Then LPCMCI is sound and complete, i.e., it returns the PAG \(\overline{P}(G)\).

Proof of Theorem 2. Soundness: According to the MMR orientation rule the initialization of \(C(G)\) in line 1 of Algorithm \(S1\) produces an LPCMCI-PAG \(C(G)\). Since Lemma \(S9\) proves that \(C(G)\) is still an LPCMCI-PAG after line 3, this remains true when some parentships are carried over after the re-initialization in line 4. Stationarity both with respect to orientations and adjacencies is always enforced by construction. The statement then follows from Lemmas \(S9\) and \(S11\) together with the
We find that also here adjacency and orientation recall are much higher in LPCMCI as compared to
2 with shape parameter
with the ParCorr CI test for varying number of variables, maximum time lag, sample size, and fraction
whether a node is in a separating sets are made in an order-independent way.

□

Theorem 3 (LPCMCI is order-independent). The output of LPCMCI does not depend on the order of
the N time series variables X (the j-indices may be permuted).

Proof of Theorem 3: Both Algorithms S2 and S3 remove edges only after the for-loop over ordered
pairs has been completed. The ordering of ordered pairs imposed by the outer for-loop is order-
independent. Note that the sets S search, S search, and S search are ordered by means of \( I_{\text{min}} \). Since
this is an order-independent ordering, the break commands do not introduce order-dependence. The
application of orientation rules is order-independent by construction of Algorithm S3. Orientations
and removals are only applied once the rule has been exhaustively applied, and conflicts are removed
by means of the conflict mark ‘x’. Lastly, as discussed at the end of Sec. S5 also the decision of
whether a node is in a separating sets are made in an order-independent way.

□

S8 Further numerical experiments

On the following pages we provide results for the GPDC CI test and further numerical experiments
with the ParCorr CI test for varying number of variables, maximum time lag, sample size, and fraction
of unobserved variables. For each setup we show significance levels \( \alpha = 0.01, 0.05 \) and different
autocorrelation values, numbers of variables, and sample sizes (depending on the setup). We focus
the discussion on orientation recall and precision, runtimes, and control of false positives.

Nonlinear experiments with GPDC CI test: Results for the nonlinear CI test GPDC [Runge et al., 2019b]
are shown in Figures S2 \((T = 200)\) and S3 \((T = 400)\). Each figure depicts the results \( N = 3, 5, 10 \) and \( \alpha = 0.01, 0.05 \) with varying autocorrelation on the x-axis. Note
that here we employ a numerical setup for the model in eq.[3] that features half linear and half nonlinear
dependent functions of the type \( f(x) = (1 + 5xe^{-x^2/20})x \), chosen because these tend to yield stationary
dynamics. Further, a third of the noise distributions are randomly chosen to be Weibull distributions
with shape parameter 2.

We find that also here adjacency and orientation recall are much higher in LPCMCI as compared to
FCI and RFCI, especially for contemporaneous links. Precision is overall comparable, but lagged
precision often higher for LPCMCI. For \( N = 3 \) we observe partially not controlled false positives for
all methods.

Linear experiments for varying number of variables N: In Figures S4-S6 we depict results for
varying number of variables \( N \) and \( T = 200, 500, 1000 \), \( \alpha = 0.5, 0.95, 0.99 \), and \( \alpha = 0.01, 0.05 \).
For the case of no autocorrelation LPCMCI has slightly higher recall and slightly lower precision at a
higher runtime. For intermediate autocorrelation (\( \alpha = 0.5 \)) the results are similar to those for \( \alpha = 0, \)
but FCI’s runtime is higher. For \( N = 3, T = 200, \alpha = 0.01 \) false positives are not controlled, less so
for LPCMCI. For higher autocorrelation LPCMCI has 0.2-0.4 higher contemporaneous recall and
also substantially higher lagged recall throughout. In the highly autocorrelated regime we observe
inflated false positives for FCI and RFCI due to ill-calibrated CI tests, similar to the PC algorithm as discussed in [Runge et al., 2019b].

Linear experiments for varying maximum time lag \( \tau_{\text{max}} \): In Figures S7-S9 we depict results for
varying maximum time lag \( \tau_{\text{max}} \) and \( T = 200, 500, 1000 \), \( \alpha = 0.01, 0.05 \). For no autocorrelation all methods have almost constant contemporaneous recall, only lagged
recall shows a slight decay. Note that the true PAG changes for larger maximum time lag \( \tau_{\text{max}} \). Contemporaneous precision is also largely constant, while lagged precision decreases for all methods.
Runtime increases and sharply rises for LPCMCI with \( k = 0 \), indicating that the edge removal phase of Alg. S3 is faster for a higher \( k \), i.e., after several preliminary phases have been run. FCI similarly features exploding runtimes for large \( \tau_{\text{max}} \) for both intermediate and higher autocorrelations. Again, false positives in FCI and RFCI are not well controlled for small \( \tau_{\text{max}} \) and \( \alpha = 0.01 \).
Linear experiments for varying sample size $T$: In Figures S10-S12 we depict results for varying sample size $T$ and $N = 3, 5, 10$, $a = 0, 0.5, 0.95, 0.99$, and $\alpha = 0.01, 0.05$. As expected, both recall and precision increase. Also runtime increases, but only slowly, except for LPCMCI $k = 0$ where it explodes for $N = 10$. The higher the autocorrelation, the better the increase in recall and precision for contemporaneous links. Lack of false positive control (less so for LCPCMI) is visible for all sample sizes for $N = 3$.

Linear experiments for varying the fraction of unobserved variables $\lambda$: In Figures S13-S18 we depict results for varying fractions of unobserved variables $\lambda$ and $T = 200, 500, 1000$, $N = 3, 5, 10$, $a = 0, 0.5, 0.95, 0.99$, and $\alpha = 0.01, 0.05$. For no autocorrelation both recall and precision decay, while runtime is almost constant. For intermediate and strong autocorrelation we observe a strong decay in recall (even stronger for contemporaneous links), and a less stronger decay in precision. Runtime is almost constant.
Figure S2: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with GPDC CI test [Runge et al., 2019b]) for varying autocorrelation $\alpha$ for $T = 200$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for $N = 3, 5, 10$ (top and bottom). All parameters are indicated in the upper right of each panel.
Figure S3: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with GPDC CI test [Runge et al., 2019b]) for varying autocorrelation $\alpha$ for $T = 400$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for $N = 3, 5, 10$ (top and bottom). All parameters are indicated in the upper right of each panel.
Figure S4: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying number of variables $N$ for $T = 200$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel. Some experiments did not converge within 24hrs and are not shown.
Figure S5: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying number of variables $N$ for $T = 500$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel. Some experiments did not converge within 24hrs and are not shown.
Figure S6: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying number of variables $N$ for $T = 1000$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel. Some experiments did not converge within 24hrs and are not shown.
Figure S7: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying maximum time lag $\tau_{\text{max}}$ for $T = 200$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S8: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying maximum time lag $\tau_{\text{max}}$ for $T = 500$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S9: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying maximum time lag $\tau_{\text{max}}$ for $T = 1000$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S10: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying sample size $T$ for $N = 3$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S11: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying sample size $T$ for $N = 5$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S12: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying sample size $T$ for $N = 10$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S13: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying fraction of unobserved variables $\lambda$ for $T = 200$ and $N = 5$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S14: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying fraction of unobserved variables $\lambda$ for $T = 500$ and $N = 5$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S15: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying fraction of unobserved variables $\lambda$ for $T = 1000$ and $N = 5$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S16: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying fraction of unobserved variables $\lambda$ for $T = 200$ and $N = 10$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S17: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying fraction of unobserved variables $\lambda$ for $T = 500$ and $N = 10$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
Figure S18: Results of numerical experiments for LPCMCI compared to FCI and RFCI (all with ParCorr CI test) for varying fraction of unobserved variables $\lambda$ for $T = 1000$ and $N = 10$. The left (right) column shows results for significance level $\alpha = 0.01$ ($\alpha = 0.05$). The rows depict results for increasing autocorrelation (top to bottom). All parameters are indicated in the upper right of each panel.
In Sec. S5 it was mentioned that FCI becomes non-complete when its orientation rules in the final orientation phase are modified according to the majority rule of [Colombo and Maathuis, 2014]. While this is probably known, we have not found it spelled out in the literature. Therefore, we here illustrate this point by the example given in Fig. S19.

The left and middle part of the figure respectively show the true MAG and its fully informative PAG. As proven in [Zhang, 2008], the latter will be found by the standard FCI algorithm without modification according to the majority rule. Note that the two heads at node F are put by the collider rule R0: Since F is not in the separating set $S_{DE} = \{A, B, C\}$ of D and E, the unshielded triple $D \leftarrow F \rightarrow E$ is oriented as collider $D \rightarrow F \leftarrow E$. The output of FCI with modification according to the majority rule is shown in the right part of the figure. There, the two heads at F are not found. The reason is that the majority rule instructs R0 to base its decision of whether $D \leftarrow F \rightarrow E$ is oriented as a collider not on the separating set found during the removal phases (this is $S_{DE}$) but rather on a majority vote of all separating sets of D and E in the adjacencies of D and E. However, in the example there are no such separating sets since neither D nor E is adjacent to A. Therefore, $D \leftarrow F \rightarrow E$ is not oriented as collider by R0 but rather marked as ambiguous. The heads can also not be found by R2, R3 and R4, the other rules for putting invariant heads, because these only oriented edges that are part of a triangle. Since neither $F \rightarrow D$ nor $F \rightarrow E$ is part of a triangle, the orientations are not found. As described at the end of Sec. S5 we employ a modified majority rule in LPCMCI to guarantee both completeness and order-independence.