On the Identifiability of the Post-Nonlinear Causal Model

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Abstract

By taking into account the nonlinear effect of the cause, the inner noise effect, and the measurement distortion effect in the observed variables, the post-nonlinear (PNL) causal model has demonstrated its excellent performance in distinguishing the cause from effect. However, its identifiability has not been properly addressed, and how to apply it in the case of more than two variables is also a problem. In this paper, we conduct a systematic investigation on its identifiability in the two-variable case. We show that this model is identifiable in most cases; by enumerating all possible situations in which the model is not identifiable, we provide sufficient conditions for its identifiability. Simulations are given to support the theoretical results. Moreover, in the case of more than two variables, we show that the whole causal structure can be found by applying the PNL causal model to each structure in the Markov equivalent class and testing if the disturbance is independent of the direct causes for each variable. In this way the exhaustive search over all possible causal structures is avoided.

1 INTRODUCTION

Traditionally, causal discovery algorithms, which may be constraint-based or score-based, produce a Markov equivalent class of the causal models, in which some causal directions may be undetermined (Spirtes et al., 2001; Pearl, 2000). On the other hand, a functional causal model, which expresses each variable as a function of its direct causes and the independent disturbance (Pearl, 2000), if well specified, can explain the data generating process and help find all causal relations among the variables. For example, under the condition that causal relations are linear and acyclic, the non-Gaussianity of the disturbances could help find the whole causal model uniquely (Shimizu et al., 2006), by resorting to the independent component analysis (ICA) technique (Hyvärinen et al., 2001). However, if the assumed functional causal model is not capable of approximating the true data generating process, the results may be misleading. Therefore, if the specific knowledge about the data generating mechanism is not available, to make it useful in practice, the assumed causal model should be general enough, such that it can reveal the data generating processes approximately; at the same time, the model should be identifiable, i.e., it is asymmetrical in causes and effects and is capable of distinguishing between them.

Although the linearity assumption greatly simplifies causal analysis, in some situations nonlinear effects in the system are not negligible. In particular, the recently proposed post-nonlinear (PNL) causal model takes into account the nonlinear effect of the causes, the noise effect, and sensor or measurement nonlinear distortion in the observed variables (Zhang & Hyvärinen, 2008). Mathematically, with the causal structure represented by a directed acyclic graph (DAG), it expresses each variable x_i as

$$x_i = f_{i,2}(f_{i,1}(pa_i) + e_i), \quad i = 1, ..., n, \tag{1}$$

where pa_i contains the direct causes of x_i, $f_{i,1}$ denotes the nonlinear effect of the causes, e_i is the independent disturbance, and $f_{i,2}$ denotes invertible post-nonlinear distortion in variable x_i. It includes the so-called additive noise model (Hoyer et al., 2009) as a special case in which the nonlinear distortion $f_{i,2}$ does not exist. It is also related to the idea of causal reasoning based on evaluating the complexity of conditional densities (Sun et al., 2008), since it intrinsically admits a simple expression for the conditional density of the effect given the causes. This model has been used to distinguish between causes and effects for the "Cause-effect pairs" task (Mooij et al., 2008) in the second causality challenge, and gave clearly the best results (the identified causal directions are correct for all eight data sets). Its good performance is partially due to the allowance of the measurement distortion $f_{i,2}$, which is frequently encountered in practice.

Despite its success in solving some real-world problems, there are two unsolved problems related to the PNL causal model, and they are addressed in this paper. One is the identifiability, a crucial issue, of this model. Although it was supported by empirical results and was touched in Zhang and Hyvärinen (2008), it is far from complete. Here we give a systematical investigation of its identifiability in the two-variable case, under the assumption that the density of the disturbance has an unbounded support. We show that the model is generally identifiable, and give all the non-identifiable cases, some of which are illustrated by simulation studies. Our results also have some by-products. Previously, Zhang and Hyvärinen (2008) investigated this issue, by relating this model to the PNL mixing ICA problem (Achard & Jutten, 2005), under the constraint that the nonlinear effect of the cause, $f_{i,1}$, is invertible. Our findings reveal that their results are not precise, and further provide counterexamples to the separability theorem of the PNL mixing ICA problem reported in Achard and Jutten (2005), which their results are based on. This finding may also be of interest to the ICA community, since PNL mixing ICA is an important and widely used nonlinear ICA model. In addition, our results on the identifiability of the PNL causal model also apply to the additive noise model (Hoyer et al., 2009), since the latter model is a special case of the former one.

The other problem is how to find the causal relations among more than two variables implied by this model. One may search all possible causal structures and test if they are consistent with the data in a brute-force way, but it involves high computational load and becomes impractical as the variable number increases. We provide some fundamental results for this issue. It is shown that causal discovery based on the PNL causal model for more than two variables can be achieved in two steps: after obtaining the equivalent class, one can identify the undetermined causal relations by applying this model to the causal structures in the equivalent class and testing if each disturbance is independent of the parents associated with the same variable. Consequently, the search space is greatly reduced, and statistical tests of mutual independence between more than two variables are avoided.

2 IDENTIFIABILITY

In this section we focus on the two-variable case. We investigate the identifiability of the PNL causal model, in particular, its direction, by a proof by contradiction. We assume the causal model holds in both directions $x_1 \to x_2$ and $x_2 \to x_1$, and show that this implies some very strong conditions on the distributions and functions involved in the model.

Assume that the data (x_1, x_2) are generated by the post-nonlinear (PNL) causal model with the the causal relation $x_1 \to x_2$. This data generating process can be described as

$$x_2 = f_2(f_1(x_1) + e_2), \qquad (2)$$

where x_1 and e_2 are independent, function f_1 is non-constant, and f_2 is invertible. If the other causal direction, $x_2 \to x_1$ is true, the data generating process given by the PNL causal model is

$$x_1 = g_2(g_1(x_2) + e_1), \qquad (3)$$

where x_2 and e_1 are independent, g_1 is non-constant, and g_2 is invertible.

Notation. The following notations are used hereafter. Suppose that both (2) and (3) hold. Random variables t_1 and z_2 and functions h and h_1 defined as follows:

$$\begin{aligned} t_1 &\triangleq g_2^{-1}(x_1), \quad & z_2 &\triangleq f_2^{-1}(x_2), \\ h &\triangleq f_1 \circ g_2, \quad & h_1 &\triangleq g_1 \circ f_2. \end{aligned}$$

That is, $h(t_1) = f_1(g_2(t_1)) = f_1(x_1)$, and similarly, h_1 is a function of z_2. Moreover, we let $\eta_1(t_1) \triangleq \log p_{t_1}(t_1)$, and $\eta_2(e_2) \triangleq \log p_{e_2}(e_2)$.[1] The following theorem gives the constraint that p_{t_1}, p_{e_2}, and h must satisfy to make both (2) and (3) hold.

Theorem 1 *Assume that (x_1, x_2) can be described by both of the causal relations given in (2) and in (3). Further suppose that involved densities and nonlinear functions p_{t_1}, p_{e_2}, f_1, f_2, g_1, and g_2 are third-order differentiable, and that p_{e_2} is positive on $(-\infty, +\infty)$. We then have the following equation for every (x_1, x_2) satisfying $\eta_2'' h' \neq 0$:*

$$\begin{aligned} \eta_1''' - \frac{\eta_1'' h''}{h'} &= \Big(\frac{\eta_2' \eta_2'''}{\eta_2''} - 2\eta_2''\Big) \cdot h' h'' - \frac{\eta_2'''}{\eta_2''} \cdot h' \eta_1'' \\ &\quad + \eta_2' \cdot \Big(h''' - \frac{h''^2}{h'}\Big), \end{aligned} \qquad (4)$$

and h_1 depends on η_1, η_2, and h in the following way:

$$\frac{1}{h_1'} = \frac{\eta_1'' + \eta_2'' h'^2 - \eta_2' h''}{\eta_2'' h'}. \qquad (5)$$

See Appendix for its proof. In the special case with f_2 and g_2 being the identity mapping, the above theorem becomes Theorem 1 in Hoyer et al. (2009), which was

[1] For the sake of conciseness, sometimes we drop the arguments of the functions in the presentation.

given for the additive noise model. In general, it is not obvious if Theorem 1 holds for a practical problem. Therefore, below we provide conditions which are easy to verify, by investigating (4) in Theorem 1. To this end, we first give some definitions and lemmas.

Definition 2 *The density of the continuous variable v, denoted by p_v, is said to be* log-mixed-linear-and-exponential (log-mix-lin-exp) *if it is of the form $\log p_v = c_1 e^{c_2 v} + c_3 v + c_4$, where c_1, c_2, c_3, and c_4 are constants. Clearly, to make p_v a valid density, we have $c_1 < 0$ and $c_2 c_3 > 0$. This type of distributions includes the Type-1 Gumbel distribution as a special case when $c_2 = c_3$.*

Definition 3 *The density p_v is said to be* a generalized mixture of two exponentials *if $p_v \propto (c_1 e^{c_2 v} + c_3 e^{c_4 v})^{c_5}$, with constants c_i, or equivalently, if $\log p_v = d_1 v + d_2 \log(d_3 + d_4 e^{d_5 v}) + d_6$, with constant d_i.*

Definition 4 *The density p_v is said to be* one-sided asymptotically exponential, *if $(\log p_v)' \to c$, as $v \to -\infty$ or as $v \to +\infty$, where c is a non-zero constant. It is said to be* two-sided asymptotically exponential *if $(\log p_v)' \to c_1$, as $v \to -\infty$, and $(\log p_v)' \to c_2$, as $v \to +\infty$, where c_1 and c_2 are non-zero constants.*

Clearly, log-mix-lin-exp densities are special cases of the one-sided asymptotically exponential densities, and two-sided asymptotically exponential densities include those generalized mixtures of two exponentials. Now we give a lemma to characterize some properties of a density function or its logarithm.

Lemma 5 *Suppose the density p_v is differentiable on $(-\infty, +\infty)$ and monotonic for sufficiently large v. We have the following. (i) If p_v is positive on $(-\infty, +\infty)$, then $\log p_v \to -\infty$ as $|v| \to +\infty$. (ii) If there only exists one point, denoted by $v = C$, satisfying $(\log p_v)' = 0$, then on the support of p_v, $(\log p_v)' > 0$ for $v < C$, and $(\log p_v)' < 0$ for $v > C$.*

This lemma is obvious and proof is skipped. The following lemmas discuss some special and simple solutions to (4) in Theorem 1.

Lemma 6 *Under the assumptions made in Theorem 1, if e_2 is Gaussian, then h is linear and t_1 is also Gaussian.*

Lemma 7 *Under the assumptions made in Theorem 1, if function $h = f_1 \circ g_2$ is linear, one of the following must be true:*

i. t_1 and e_2 are both Gaussian, and h_1 is also linear.

ii. The densities of t_1 and e_2 are log-mix-lin-exp, $h_1'(z_2)$ is strictly monotonic, and $h_1'(z_2) \to 0$, as $z_2 \to +\infty$ or as $z_2 \to -\infty$.

For proofs, see Appendix. We now give Theorem 8 to consider all the situations in which the PNL causal model is not identifiable.

Theorem 8 *Suppose that $\eta_2'' h' \neq 0$ at every point or that it is zero at only some discrete points. Under the assumptions made in Theorem 1, we have that p_{e_2} and p_{t_1}, as well as h, must satisfy one of the five conditions listed in Table 1.*[2]

The proof is rather long and complicated, so we just give the basic idea and its outline; see Appendix. When the nonlinear distortions f_2 and g_2 are constrained to be the identity mapping, this result also applies to the identifiability of the additive noise model. We give the following remarks on the situations listed in Table 1. Situation I in Table 1 is the linear Gaussian case, which is well know to be not identifiable. Situations II∼V are novel. As discussed in Zhang and Hyvärinen (2008), if f_1 is constrained to be invertible, the PNL causal model (2) can be transformed to the PNL mixing ICA model (Achard & Jutten, 2005), with $f_1(x_1)$ and e_2 considered as sources. The identifiability of the former model is then implied by the separability of the latter one. Previously, under weak conditions, it was shown that the PNL mixing ICA model is separable if at most one of the sources is Gaussian (Achard & Jutten, 2005). In Situations II∼V, p_{e_2} is not Gaussian, but the causal model is not identifiable, and consequently the corresponding PNL mixing ICA model is not separable. This means that the established separability results of the PNL mixing ICA problem have some flaws and require further investigation.

Below we give some corollaries which follow from Theorem 8. They can be easily exploited to examine if the causal relation between two variables is unique. The following assumptions are made in the corollaries.

A1. The data (x_1, x_2) are generated by the PNL causal model (2), with f_1 and f_2 being third-order differentiable.

A2. Densities p_{e_2} and p_{x_1} are third-order differentiable, p_{e_2} is positive on $(-\infty, +\infty)$, and $\eta_2'' = (\log p_{e_2})''$ is zero at most at some discrete points.

The following corollary immediately follows Theorem 8, so its proof is skipped.

[2]Note that the identifiability of the PNL causal model (2) depends directly on the distribution of t_1 and e_2, instead of the distribution of the observed variables x_1 and x_2.

Table 1: All situations in which the PNL causal model is not identifiable.

	p_{e_2}	p_{t_1} $(t_1 = g_2^{-1}(x_1))$	$h = f_1 \circ g_2$	Remark
I	Gaussian	Gaussian	linear	h_1 also linear
II	log-mix-lin-exp	log-mix-lin-exp	linear	h_1 strictly monotonic, and $h_1' \to 0$, as $z_2 \to +\infty$ or as $z_2 \to -\infty$
III	log-mix-lin-exp	one-sided asymptotically exponential (but not log-mix-lin-exp)	h strictly monotonic, and $h' \to 0$, as $t_1 \to +\infty$ or as $t_1 \to -\infty$	—
IV	log-mix-lin-exp	generalized mixture of two exponentials	Same as above	—
V	generalized mixture of two exponentials	two-sided asymptotically exponential	Same as above	—

Corollary 9 *Suppose that assumptions A1 & A2 hold. If p_{e_2}, the density of the disturbance, is not Gaussian, nor log-mix-lin-exp, nor a generalized mixture of two exponentials, then the PNL causal model (2) is identifiable.*

Corollary 10 considers the identifiability of the PNL causal model with f_1, the nonlinear effect of the cause, being non-invertible.

Corollary 10 *Suppose that assumptions A1 & A2 hold. If function f_1 is not invertible, then the PNL causal model (2) is identifiable.*

For proof, see Appendix. This result is intuitively appealing, and confirms the finding in Friedman and Nachman (2000).

3 NONLINEAR ICA-BASED IDENTIFICATION METHOD

If data (x_1, x_2) follow the PNL causal model with causal direction $x_1 \to x_2$, from (2), we can see that the disturbance e_2, which is independent from x_1, can be expressed in terms of x_1 and x_2:

$$e_2 = f_2^{-1}(x_2) - f_1(x_1).$$

This provides a way to verify if $x_1 \to x_2$ holds according to the PNL causal model, as given below.

Under the hypothesis $x_1 \to x_2$, we can estimate the disturbance e_2 by finding functions l_1 and l_2 such that $\hat{e}_2 = l_2(x_2) - l_1(x_1)$ is independent from x_1. This is then a constrained nonlinear ICA problem, and can be achieved by minimizing $I(x_1, \hat{e}_2)$, the mutual information between x_1 and $\hat{e}_2$ (Zhang & Hyvärinen, 2008). After some simplifications, one can see $I(x_1, \hat{e}_2) = -E \log p_{\hat{e}_2}(\hat{e}_2) - E \log |l_2'(x_2)| + H(x_1) - H(x_1, x_2)$. As the last two terms do not depends on $l_1(x_1)$ and $l_2(x_2)$, minimizing $I(x_1, \hat{e}_2)$ is equivalent to maximizing $E \log p_{\hat{e}_2}(\hat{e}_2) + E \log |l_2'(x_2)|$. Following Zhang and Hyvärinen (2008), we use multi-layer perceptrons (MLP's) to represent l_1 and l_2. The involved parameters can then be learned by gradient-based methods. Finally, if statistical independence tests, such as the kernel-based test (Gretton et al., 2008), confirm that $\hat{e}_2$ is independent from x_1, $x_1 \to x_2$ is supported by the PNL causal model, and the learned l_1 and l_2 provide an estimate of f_1 and f_2^{-1}, respectively.

To find the causal relation between x_1 and x_2 implied by the PNL causal model, one needs to test both hypotheses $x_1 \to x_2$ and $x_2 \to x_1$, using the method just described. If exactly one of them holds, the causal relation between x_1 and x_2 implied by the PNL model has been successfully found. If neither of them holds, there is no PNL causal relation between x_1 and x_2. If both hold, the cause and effect could not be distinguished by the PNL causal model; additional information, such as the smoothness of the involved nonlinearities, may help find the causal model with a lower complexity.

4 MORE THAN TWO VARIABLES

The PNL acyclic causal model (1) is applicable in the case of more than two variables. When there are only very few variables, one may use a brute-force search to find the causal relations, like the estimation of the additive noise model in Hoyer et al. (2009); for each possible acyclic causal structure, represented by a DAG, we use the nonlinear ICA-based approach to estimate the corresponding disturbances, and then verify if they are mutually independent by performing independence tests. The simplest causal model which gives independent disturbances is preferred. Clearly this approach may encounter two difficulties. One is that the test of mutual independence is difficult to do when we have many variables. The other is that the search space of all possible DAG's increases too rapidly with the variable number. Consequently, this approach involves high computational load, and does not scale well with the number of variables.

A more practical approach to finding the causal relations implied by the PNL causal model consists of the following two steps. We first use conditional independence-based methods to find the d-separation equivalent class. Next, the PNL causal model is used to identify the causal directions that cannot be determined in the first step: for each causal structure contained in the equivalent class, we estimate the disturbances, and determine if this causal structure is plausible, by examining if the disturbance in a variable x_i is independent from the parents of x_i. Consequently, one avoids the exhaustive search over all possible causal structures and high-dimensional statistical tests of mutual independence. The validity of this approach is supported by the following theorem.

Theorem 11 *When fitting variables $x_1, ..., x_n$ to the PNL acyclic causal model (1) with the causal structure represented by the DAG $\mathcal{G}$, the disturbances e_i are mutually independent if and only if the causal Markov condition holds (i.e., each variable x_i is independent of its non-descendants conditional on its parents pa_i in $\mathcal{G}$), and the disturbance e_i in x_i is independent of the parents of x_i.*

Proof is given in Appendix. An important issue in this approach is how to perform conditional independence tests for variables with nonlinear causal relations. Generally speaking, the results of nonparametric conditional independence tests may be unreliable when the conditional set contains many variables, due to the curse of dimensionality. Traditionally, in the implementation of most conditional independence-based causal discovery algorithms, such as PC (Spirtes et al., 2001) and IC (Verma & Pearl, 1990), it is assumed that the variables are either discrete or Gaussian with linear causal relations. Although this assumption greatly simplifies the difficulty in conditional independent tests, it usually does not hold in our case which involves nonlinear causal effects and non-Gaussian variables. Alternatively, in our case, one may simplify the conditional independence test procedure by making use of the particular structure of the PNL causal model. This is out of the scope of this paper and left for future work.

5 SIMULATIONS

The PNL causal model has been applied for causal discovery of two variables with real-world data in Zhang and Hyvärinen (2008). It successfully identified the causal directions for all eight data sets in the "Cause-effect pairs" task (Mooij et al., 2008) included in Causality Challenge #2, without any background knowledge. This demonstrated the practical usefulness of this model and the identification method for some real-world problems. Here we conduct simulations to verify the non-identifiable conditions of this model with two variables, given in Theorem 8. In particular, Situation I in Table 1 is well known to be not identifiable, but the others are completely new and interesting. Here we use illustrative examples to show the non-identifiability in Situations II and V.

5.1 ON SITUATION II IN TABLE 1

In Situation II in Table 1, function $h = f_1 \circ g_2$ is linear and the densities of t_1 and e_2 are log-mix-lin-exp (given by (10) and (9) in Appendix, respectively), and the PNL causal model is not identifiable. To illustrate that, one just needs to confirm that t_1 and z_2 are independent of e_2 and e_1, respectively; independence between t_1 and e_2 means that the causal relation $x_1 \rightarrow x_2$ holds, as described by (2); in addition, if z_2 and e_1 given by (6) and (7) (see Appendix) are also independent, one can see that $x_2 \rightarrow x_1$ also holds, and that the PNL model is not identifiable.

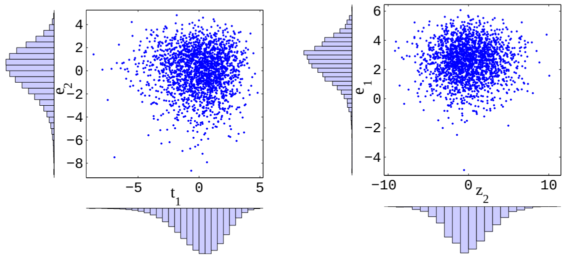
Given c_1, c_2, c_3, and c_5 in (10) and (9), one can find the constants c_4 and c_7 such that $p_{t_1} = e^{\eta_1}$ and $p_{e_2} = e^{\eta_2}$ are valid densities. We then generate random numbers as realizations of the independent variables t_1 and e_2, by applying the inverse of their cumulative distribution functions (CDF's) to independent and uniformly distributed variables. According to (7), variable z_2 involved in the causal relation $x_2 \rightarrow x_1$ is calculated as $z_2 = e_2 + h(t_1)$. The other variable, e_1, can be found according to (6), if h_1 is known. According to (11), we have

$$h_1' = e^{c_1 z_2 - c_5 + c_2} \Big/ \Big(\frac{1}{h'} + h' e^{c_1 z_2 - c_5 + c_2} \Big).$$

This yields $h_1 = \frac{1}{h' c_1} \log | \frac{1}{h'} + h' e^{c_1 z_2 - c_5 + c_2} | + c_8$, where c_8 is an arbitrary constant. Substituting h_1 into (6), we can find e_1.

In our simulation study, we set $h(t_1) = -t_1$, $c_1 = 0.3$, $c_2 = -1$, $c_3 = 1$, $c_5 = -1$ $c_8 = 0$, and variables t_1 and e_2 were made zero-mean. 2000 samples were drawn. Fig. 1 (a) gives the scatter plot of t_1 and e_2, as well as their marginal histograms. Finally, the scatter plot of z_2 and e_1 is shown in Fig. 1 (b). To verify if z_2 and e_1 are independent, we conducted the kernel-based statistical independence tests (Gretton et al., 2008). The left part of Table 2 presents the independence test results for the pairs (t_1, e_2) and (z_2, e_1). For both pairs, The independence hypothesis is accepted at the significance level $\alpha = 0.05$. That is, in this situation, the PNL causal model cannot distinguish the cause from effect, if we do not have further knowledge about the data generating process.

We further generated observed data (x_1, x_2) from variables t_1 and e_2, aiming to verify if the nonlinear ICA-based identification method can detect both causal



(a) (b)

Figure 1: (a) Scatter plot of $t_1 = g_2^{-1}(x_1)$ and e_2 in Simulation 1. (b) That of $z_2 = f_2^{-1}(x_2)$ and e_1.

Table 2: Result of kernel-based independence tests in Simulation 1, at the significance level $\alpha = 0.05$. The independence hypothesis is accepted in all the four cases. See main text for further explanations.

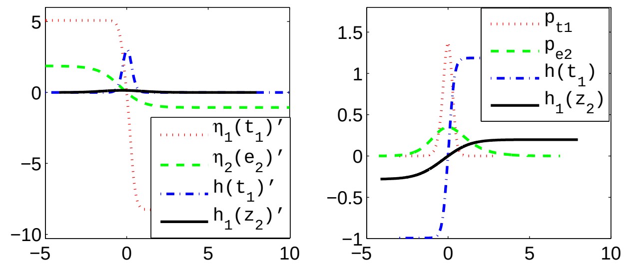
	t_1&e_2	z_2&e_1	x_1&$\hat{e}_2$	x_2&$\hat{e}_1$
Threshold	0.5669	0.5665	0.4347	0.5778
Statistic	0.3497	0.1226	0.1430	0.1842

directions. Note that the identifiability of the PNL causal model only depends the distributions of t_1 and e_2 and function $h(t_1) = f_1(g_2(t_1))$. In situation II in Table 1, f_1, f_2, and g_2 can be arbitrary, given that $h = f_1 \circ g_2$ satisfies the condition.[3] In this simulation, we let $g_2(t_1) = t_1/2 + t_1^{1/3}$; since $h = f_1 \circ g_2$, f_1 was then constructed as $f_1 = h \circ g_2^{-1}$. we let $f_2(h(t_1)+e_2) = \tanh((h(t_1)+e_2)/8)$. Finally, (x_1, x_2) were constructed from t_1 and e_2 by $x_1 = g_2(t_1)$ and (2). We applied the nonlinear ICA-based method given in Section 3, and obtained $\hat{e}_2$ and $\hat{e}_1$, which are the estimate of the disturbance under the hypotheses $x_1 \rightarrow x_2$ and $x_2 \rightarrow x_1$, respectively. The right part of Table 2 reports the results of independence tests for the pairs $(x_1, \hat{e}_2)$ and $(x_2, \hat{e}_2)$. Both pairs accept the independence hypothesis, meaning that both the estimated PNL causal model with $x_1 \rightarrow x_2$ and that with $x_2 \rightarrow x_1$ can explain the data.

5.2 ON SITUATION V IN TABLE 1

We next verify Situation V in Table 1. In the proof of Theorem 8, Solution 1 to the functional equation (12), given by (14), with the constraints $A_3 = -A_2$ and $A_4 \neq 0$, results in this situation. Generally speaking, in this situation, the solutions of η_1 and h cannot be expressed in terms of elementary functions. We then found numerical solutions of η_1', h', and η_2' to the overdetermined system of ordinary differential equations (ODE's) given in (14) using MATLAB. We let $A_1 = 2$, $A_2 = 0.4$, $A_4 = 1$, $c_6 = -10$, $c_7 = 1.6$, and the initial conditions are $\eta_1'(t_1 = 0) = 0$, $\eta_2'(e_2 = 0) = 0$, $h'(t_1 = 0) = 3$. The solutions of η_1', h', and η_2' are depicted in Fig. 2(a). One can see that h' is clearly close to zero for large t_1, consistent with Situation V. Furthermore, we set $h(t_1 = 0) = 0$, and obtained the solutions of h; also noting that the total integral of $p_{t_1} = e_1^{\eta}$ and $p_{e_2} = e^{\eta_2}$ is one, finally we obtained the solutions of η_1, h, and η_2, as plotted in Fig. 2(b).

[3]Note that if f_1 is not invertible, the causal model is always identifiable; see Corollary 10.

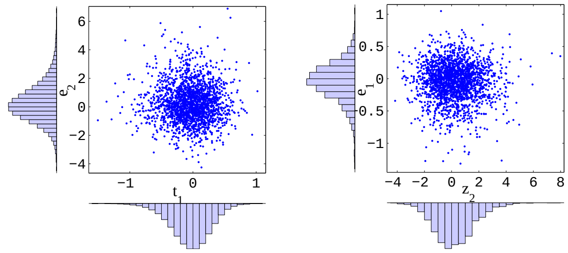


(a) (b)

Figure 2: An example of Situation V in Table 1. (a) The curves of $\eta_1(t_1)'$, $\eta_2(e_2)'$, $h(t_1)'$, and $h_1(z_2)'$. $\eta_1(t_1)'$, $\eta_2(e_2)'$, and $h(t_1)'$ were obtained by solving the system of ODE's in (14) numerically. $h_1(t_1)'$ was given by (5). (b) The curves of $p_{t_1} = e^{\eta_1}$, $p_{e_2} = e^{\eta_2}$, $h(t_1)$, and $h_1(z_2)$. See main text for detailed explanations.

We used radial basis networks (RBF's) to learn the probability density functions (PDF's) of t_1 and e_2 from their numerical values, and then drew random samples of t_1 and e_2 by applying the inverse of their CDF's to independent and uniformly distributed variables. Fig. 3(a) gives the scatter plot of t_1 and e_2 used in this simulation and their marginal histograms. After that, we aimed to find variables z_2 and e_1, which are involved in the causal relation $x_2 \rightarrow x_1$, by making use of the transformation given in (6) and (7). Apparently, $z_2 = h(t_1) + e_2$. In order to find variable e_1, one needs to find $h_1(z_2)$. We first calculated $h_1(z_2)'$ according to (5). It is also given in Fig. 2(a), and the solution of h_1 with the initial condition $h_1(0) = 0$ is shown in Fig. 2(b). Variable e_1 is then found as $e_1 = t_1 + h_1(z_2)$. The scatter plot of z_2 and e_1 is shown in Fig. 3(b). Results of statistical independence tests, given in the left part of Table 3, confirm statistical independence between t_1 and e_2 and that between z_2 and e_1.

Analogously to Simulation I, we constructed observable data (x_1, x_2) from t_1, e_2, and h given above. To do that, we let $g_2(t_1) = t_1 + t_1^3$ and $f_2(h(t_1)+e_2) = \log(6 + h(t_1) + e_2)$, and f_1 was constructed as $f_1 = h \circ g_2^{-1}$. The nonlinear ICA-based method was then applied to the data (x_1, x_2). As shown in the right part of Table 3, under both hypotheses $x_1 \rightarrow x_2$ and $x_2 \rightarrow x_1$,



(a) (b)

Figure 3: (a) Scatter plot of t_1 and e_2, which are independent variables with the densities given in Fig. 2(b). (b) Scatter plot of z_2 and e_1, which were obtained by making use of the transformation in (6) and (7).

Table 3: Result of independence tests in Simulation 2 at the significance level $\alpha = 0.05$. The independence hypothesis is accepted in all the four cases.

	t_1&e_2	z_2&e_1	x_1&$\hat{e}_2$	x_2&$\hat{e}_1$
Threshold	0.5483	0.1561	0.5081	0.6912
Statistic	0.1641	0.0669	0.3011	0.4142

the assumed cause is independent from the estimate of the disturbance. Consequently, both causal directions can explain the data, and in this example the PNL causal model is not identifiable.

6 CONCLUSION

We have investigated the identifiability of the post-nonlinear (PNL) causal model in the two-variable case, and a practical identification method based on nonlinear function approximations and independence tests was discussed. Our results show that this model is generally identifiable, and consequently can be used to distinguish the cause from effect. All the particular situations in which this model is not identifiable were reported in Theorem 8, and some of them were verified and illustrated by simulations. For the situation with more than two variables, we showed that it is not necessary to apply the PNL causal model to all of the given variables directly, which becomes intractable as the variable number increase; instead, to find the whole causal structure, one can apply this causal model to the Markov equivalent class and test if the estimated disturbance is independent from the parents associated with the same variable.

Acknowledgements

The authors would like to thank Patrik Hoyer for helpful comments and suggestions.

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APPENDIX: SOME PROOFS

Proof of Theorem 1: We prove this theorem using the linear separability of the logarithm of the joint density of independent variables, which states the fact that for a set of independent random variables whose joint density is twice differentiable, the Hessian of the logarithm of their density is diagonal everywhere (Lin, 1998). Since g_2 is invertible, the independence between x_1 and e_2 is equivalent to that between t_1 and e_2. Similarly, the independence between x_2 and e_1 is equivalent to that between z_2 and e_1. Combining the two causal models (2) and (3), one can see that the transformation from (z_2, e_1) to (t_1, e_2) is

$$\begin{aligned} t_1 &= h_1(z_2) + e_1, && (6) \\ e_2 &= z_2 - h(t_1). && (7) \end{aligned}$$

Denote by $\mathbf{J}$ the Jacobian matrix of this transformation. One can see that $|\mathbf{J}| = 1$. Denote by $p_{(z_2,e_1)}$ the joint density of (z_2, e_1). We then have $p_{t_1} \cdot p_{e_2} = p_{(z_2,e_1)}/|\mathbf{J}| = p_{(z_2,e_1)}$, so, $\log p_{(z_2,e_1)} = \eta_1(t_1) + \eta_2(e_2)$. One can find the (1,2)-th entry of the Hessian matrix of $\log p_{(z_2,e_1)}$ w.r.t. (z_2, e_1): $\frac{\partial^2 \log p_{(z_2,e_1)}}{\partial e_1 \partial z_2} = \eta_1'' \frac{\partial t_1}{\partial z_2} - \eta_2'' h' \frac{\partial e_2}{\partial z_2} - \eta_2' h'' \frac{\partial t_1}{\partial z_2} = \eta_1'' h_1' - \eta_2'' h' + \eta_2'' h'^2 h_1' - \eta_2' h'' h_1'$. The independence between z_2 and e_1 implies $\frac{\partial^2 \log p_{(z_2,e_1)}}{\partial e_1 \partial z_2} = 0$ for every possible (z_2, e_1). That is, $\eta_1'' h_1' - \eta_2'' h' + \eta_2'' h'^2 h_1' - \eta_2' h'' h_1' = 0$. From this equation one can see that $h_1' = 0$ implies $\eta_2'' h' = 0$. Consequently, the points which satisfy $\eta_2'' h' \neq 0$ also make $h_1' \neq 0$. For such points, dividing both sides of this equation by $h_1' \eta_2'' h'$ finally leads to (5). Furthermore, since h_1 is a functions of z_2 and does not depend on e_1, we have $\partial\Big(\frac{1}{h_1'}\Big)\Big/\partial e_1 = 0$. According to (5), we have $\partial\Big(\frac{\eta_1'' + \eta_2'' h'^2 - \eta_2' h''}{\eta_2'' h'}\Big)/\partial e_1 = 0$, which gives $2\eta_2''^2 h'^2 h'' - \eta_2' \eta_2'' h' h''' + \eta_2'' \eta_1''' h' - \eta_2' \eta_2''' h'^2 h'' + \eta_2' \eta_2'' h''^2 + \eta_2''' \eta_1'' h'^2 - \eta_2'' \eta_1'' h'' = 0$. For the points satisfying $\eta_2'' h' \neq 0$, we divide both sides of the above equation by $\eta_2'' h'$. After some simplifications, (4) is obtained. ■

Proof of Lemma 6: Gaussianity of e_2 implies that $\eta_2''' \equiv 0$ and that η_2'' is constant. (4) then reduces to

$$\eta_1''' - \frac{\eta_1'' h''}{h'} + 2\eta_2'' \cdot h' h'' = \eta_2' \cdot \Big(h''' - \frac{h''^2}{h'}\Big). \quad (8)$$

Since the left-hand side does not depend on e_2 and η_2' is a function of e_2, we have $h''' - \frac{h''^2}{h'} = 0$, which gives $h'''/h' - \frac{h''^2}{h'^2} = 0$. That is, $(h''/h')' = 0$, so $h''/h' = c_1$. If $c_1 = 0$, h is linear, and $h'' = h''' = 0$. (8) then yields $\eta_1''' = 0$, meaning that t_1 is Gaussian.

Otherwise, $h' = \pm e^{c_1 t_2 + c_2}$. Moreover, the left-hand side of (8) must also be zero, which means $\frac{\eta_1'''}{h'} - \frac{\eta_1'' h''}{h'^2} + 2\eta_2'' h'' = 0$. By integration, it gives $\int \Big(\frac{\eta_1'''}{h'} - \frac{\eta_1'' h''}{h'^2} + 2\eta_2'' h''\Big) dt_1 = \eta_1''/h' + 2\eta_2'' h' = c_3$, so $\eta_1'' = -2\eta_2'' h'^2 + c_3 h' = -2\eta_2'' e^{2c_1 t_1 + 2c_2} \pm c_3 e^{c_1 t_1 + c_2}$. Consequently $\eta_1 = \frac{-\eta_2''}{2c_1^2} e^{2c_1 t_1 + 2c_2} \pm \frac{c_3}{c_1^2} e^{c_1 t_1 + c_2} + c_4 t_1 + c_5$. Noting that η_2'' is a negative constant, we can see that $\eta_1 \to +\infty$ when $c_1 t_1 \to +\infty$. This contradicts Lemma 5. Thus, c_1 must be zero, h is linear, and t_1 is Gaussian. ■

Proof of Lemma 7: Note that η_2'' (as well as η_1'') is not constantly zero, as a density function of e_2 could not be proportional to $e^{c_1 e_2 + c_2}$. When h is linear, h' is constant and $h'' = h''' = 0$, and (4) becomes

$$\eta_1''' = -\frac{\eta_2'''}{\eta_2''} \cdot h' \eta_1'', \text{ i.e., } \frac{\eta_1'''}{\eta_1''} = -h' \cdot \frac{\eta_2'''}{\eta_2''}$$

Since $\frac{\eta_1'''}{\eta_1''}$ and $\frac{\eta_2'''}{\eta_2''}$ depends only on t_1 and e_2, respectively, the equation above implies that both $\frac{\eta_1'''}{\eta_1''}$ and $\frac{\eta_2'''}{\eta_2''}$ are constants. Let $\frac{\eta_2'''}{\eta_2''} = c_1$, we have $\frac{\eta_1'''}{\eta_1''} = -h' c_1$. If $c_1 = 0$, clearly both e_2 and t_1 are Gaussian, and proposition (i) holds.

Otherwise, we have $\log|\eta_2''| = c_1 e_2 + c_2$. Consequently $\eta_2'' = \pm e^{c_1 e_2 + c_2}$ and $\eta_2 = \pm \frac{1}{c_1^2} e^{c_1 e_2 + c_2} + c_3 e_2 + c_4$. If $\eta_2 = \frac{1}{c_1^2} e^{c_1 e_2 + c_2} + c_3 e_2 + c_4$, clearly $\eta_2 \to +\infty$ when $\mathrm{sgn}(c_1) \cdot e_2 \to +\infty$, which contradicts Lemma 5. One can verify that when $c_1 c_3 > 0$, the solution

$$\eta_2'' = -e^{c_1 e_2 + c_2}, \text{ or } \eta_2 = -\frac{1}{c_1^2} e^{c_1 e_2 + c_2} + c_3 e_2 + c_4 \quad (9)$$

corresponds to valid densities. Analogously we have

$$\eta_1'' = -e^{-h' c_1 t_1 + c_5}, \text{ or } \eta_1 = -\frac{1}{h'^2 c_1^2} e^{-h' c_1 t_1 + c_5} + c_6 t_1 + c_7. \quad (10)$$

Thus the densities of t_1 and e_2 are both log-mix-lin-exp.

Combining (5), (9) and (10), and recalling that h is linear, we have

$$\begin{aligned} h_1' &= \frac{\eta_2'' h'}{\eta_1'' + \eta_2'' h'^2 - \eta_2' h''} = \frac{1}{\eta_1''/(\eta_2'' h') + h'} \\ &= \frac{1}{e^{-c_1 z_2 + c_5 - c_2}/h' + h'}. \quad (11) \end{aligned}$$

One can see that $h_1' \to 0$, as $\mathrm{sgn}(c_1) \cdot z_2 \to +\infty$, and as $\mathrm{sgn}(c_1) \cdot z_2 \to -\infty$, $h_1' \to h'$, which is a constant. Therefore Lemma 7 is true. ■

Outline of Proof of Theorem 8: Eq. (4) can be re-written as a bilinear functional equation (Polyanin & Zaitsev, 2004) of the form:

$$\begin{aligned} &\Phi_1(t_1)\Psi_1(e_2) + \Phi_2(t_1)\Psi_2(e_2) \\ &\quad + \Phi_3(t_1)\Psi_3(e_2) + \Phi_4(t_1)\Psi_4(e_2) = 0, \quad (12) \end{aligned}$$

where

$$\begin{array}{ll} \Phi_1(t_1) = \eta_1''' - \frac{\eta_1''h''}{h'}, & \Phi_2(t_1) = h''' - \frac{h''^2}{h'}, \\ \Phi_3(t_1) = h'h'', & \Phi_4(t_1) = h'\eta_1'', \\ \Psi_1(e_2) = -1, & \Psi_2(e_2) = \eta_2', \\ \Psi_3(e_2) = \frac{\eta_2'\eta_2'''}{\eta_2''} - 2\eta_2'', & \Psi_4(e_2) = -\frac{\eta_2'''}{\eta_2''}. \end{array} \tag{13}$$

Note that functionals $\Phi_i(t_1)$ and $\Psi_i(e_2)$ depend only on t_1 and e_2, respectively. We then find all possible situations in which (12) holds.

Clearly $\Phi_4(t_1)$, $\Psi_1(e_2)$, and $\Psi_2(e_2)$ in (13) are not constantly zero. We first consider some simple cases of the solutions to (12), with $\Phi_3(t_1) \equiv 0$, $\Psi_4(e_2) \equiv 0$, or $\Phi_2(t_1) \equiv 0$. These cases either have no valid solutions for η_1, η_2, and h, or the solutions are covered by the situations in Table 1.

When none of the functions mentioned above is constantly zero, it can be shown that the functional equation of the form (12) has three solutions, which are (Polyanin & Zaitsev, 2004)

Solution 1:

$$\begin{array}{ll} \Phi_1 = A_1\Phi_3 + A_2\Phi_4, & \Phi_2 = A_3\Phi_3 + A_4\Phi_4, \\ \Psi_3 = -A_1\Psi_1 - A_3\Psi_2, & \Psi_4 = -A_2\Psi_1 - A_4\Psi_2, \end{array} \tag{14}$$

Solution 2:

$$\begin{array}{l} \Phi_1 = B_1\Phi_3, \quad \Phi_2 = B_2\Phi_3, \quad \Phi_4 = B_3\Phi_3, \\ \Psi_3 = -B_1\Psi_1 - B_2\Psi_2 - B_3\Psi_4, \end{array} \tag{15}$$

Solution 3:

$$\begin{array}{l} \Psi_2 = C_1\Psi_1, \quad \Psi_3 = C_2\Psi_1, \quad \Psi_4 = C_3\Psi_1, \\ \Phi_1 = -C_1\Phi_2 - C_2\Phi_3 - C_3\Phi_4, \end{array} \tag{16}$$

where A_i, B_i, and C_i are arbitrary constants. Each possible solution given above is an over-determined system of ordinary differential equations (ODE's). In most cases, solutions of η_1, η_2, and h to the system, which also satisfy the properties given in Lemma 5, can be found in closed form. In the remaining cases, we use the way of phase portrait (Braun, 1993) to analyze the behavior of the solutions. We consider all possible cases, and the solutions are always covered by the five situations enumerated in Table 1. ■

Proof of Corollary 10: First, consider the case where $f_1' \neq 0$ at every point or it is zero at only some discrete points. As $h = f_1 \circ g_2$ and g_2 is invertible, $h' = 0$ holds at most at some discrete points. All the situations in which the PNL causal model is not identifiable are given in in Table 1. One can see that in all these situations, $h = f_1 \circ g_2$ is invertible. When f_1 is not invertible, no matter what g_2 is, it is impossible to make $h = f_1 \circ g_2$ invertible, i.e., none of the conditions in Table 1 holds. Consequently, in this case the causal direction between x_1 and x_2 is uniquely identified.

Next, consider the case where $f' \equiv 0$ on the domain $\mathbb{D}_0 \in \mathbb{R}$. Let C be a point between $\mathbb{D}_0$ and the domain $\mathbb{D}_n$ on which $f' = 0$ holds at most at some discrete points. Without loss of generality, we assume that $\mathbb{D}_n$ is on the right side of $\mathbb{D}_0$. As $h = f_1 \circ g_2$, we have $h(t_1 = C^-)' = 0$. Suppose that both $x_1 \to x_2$ and $x_2 \to x_1$ can explain the data. In all the situations listed in Table 1, $h' \neq 0$. Hence, $h(t_1 = C^+)' \neq 0$. As $h(t_1 = C^+)' \neq h(t_1 = C^-)$, h is not differentiable at $t_1 = C$, which causes a contradiction. So in this case the causal direction between x_1 and x_2 given by the PNL causal model is also unique. ■

Proof of Theorem 11: The necessity part is obvious, and below we prove the sufficiency part, which states that disturbances $e_1, ..., e_n$ are mutually independent, or equivalently, $x_1, ..., x_n$ follow the PNL causal model represented by $\mathcal{G}$, if the causal Markov condition holds and the disturbance e_i in the variable x_i is independent of pa_i. Let $z_i \triangleq f_{i,2}^{-1}(x_i)$. As the causal relations are acyclic, we can arrange x_i in an order such that no later variable causes any earlier one. Without loss of generality, we assume that $(x_1, x_2, ..., x_n)$ is one of such orders. For any $i = 1, ..., n$, since $x_i = f_{i,2}(z_i)$, we have $p(x_i|pa_i) = p(z_i|pa_i)/|f_{i,2}'(z_i)|$. Therefore,

$$\begin{aligned} H(e_i) &\geq H(e_i|pa_i) & (17) \\ &= H(z_i|pa_i) = -E\{\log p(z_i|pa_i)\} \\ &= -E\{\log p(x_i|pa_i)\} - E\{\log|f_{i,2}'(z_i)|\} \\ &= H(x_i|pa_i) - E\{\log|f_{i,2}'(z_i)|\} \\ &\geq H(x_i|x_1, ...x_{i-1}) - E\{\log|f_{i,2}'(z_i)|\}, & (18) \end{aligned}$$

where $H(\cdot)$ denotes the entropy, the equality in (17) holds if and only if e_i is independent from pa_i, and the equality in (18) holds if and only if the causal Markov condition holds, i.e., elements of $\{x_k | x_k \notin pa_i, 1 \leq k \leq i-1\}$ are independent of x_i given pa_i. Taking the summation of (18) over i gives

$$\begin{aligned} &\sum_i H(e_i) \\ \geq\ &\sum_i H(x_i|x_1, ..., x_{i-1}) - \sum_i E\{\log|f_{i,2}'(z_i)|\} \\ =\ &H(x_1, ..., x_n) - \sum_i E\{\log|f_{i,2}'(z_i)|\}. \end{aligned} \tag{19}$$

In addition, since e_i does not depend on x_j $(j > i)$, the Jacobian matrix of the transformation from $(x_1, ...x_n)$ to $(e_1, ...e_n)$ is lower-triangular, with the (i, i)th entry being $1/f_{i,2}'(z_i)$. Consequently, the absolute value of the determinant of this Jacobian matrix is $|\mathbf{J}| = [\Pi_i f_{i,2}'(z_i)]^{-1}$. Recalling (19), when the causal Markov condition holds and e_i is independent of pa_i, the mutual information of $e_1, ...e_n$ is then $I(e_1, ..., e_n) = \sum_i H(e_i) - H(e_1, ..., e_n) = \sum_i H(e_i) - [H(x_1, ..., x_n) + \log|\mathbf{J}|] = \sum_i H(e_i) - H(x_1, ..., x_n) + \sum_i \log|f_{i,2}'(v_i)| = 0$. That is, $e_1, ..., e_n$ are mutually independent. ■