

# Distinguishing Causes from Effects using Nonlinear Acyclic Causal Models

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## Abstract

Distinguishing causes from effects is an important problem in many areas. In this paper, we propose a very general but well defined nonlinear acyclic causal model, namely, post-nonlinear acyclic causal model with inner additive noise, to tackle this problem. In this model, each observed variable is generated by a nonlinear function of its parents, with additive noise, followed by a nonlinear distortion. The nonlinearity in the second stage takes into account the effect of sensor distortions, which are usually encountered in practice. In the two-variable case, if all the nonlinearities involved in the model are invertible, by relating the proposed model to the post-nonlinear independent component analysis (ICA) problem, we give the conditions under which the causal relation can be uniquely found. We present a two-step method, which is constrained nonlinear ICA followed by statistical independence tests, to distinguish the cause from the effect in the two-variable case. We apply this method to solve the problem “CauseEffectPairs” in the Pot-luck challenge, and successfully identify causes from effects.

**Keywords:** causal discovery, sensor distortion, additive noise, nonlinear independent component analysis, independence tests

## 1. Introduction

Given some observable variables, people often wish to know the underlying mechanism generating them, and in particular, how they are influenced by others. Causal discovery has attracted much interest in various areas, such as philosophy, psychology, machine learning, etc. There are some well-known algorithms for causal discovery. For example, conditional independence tests can be exploited to remove unnecessary connections among the observed variables and to produce a set of acyclic causal models which are in the  $d$ -separation equivalence class (Pearl, 2000; Spirtes et al., 2000).

Recently, some methods have been proposed for model-based causal discovery of continuous variables (see, e.g., Shimizu et al., 2006; Granger, 1980). Model-based causal discovery

assumes a generative model to explain the data generating process. If the assumed model is close to the true one, such methods could not only detect the causal relations, but also discover the form in which each variable is influenced by others. For example, Granger causality assumes that effects must follow causes and that the causal effects are linear (Granger, 1980). If the data are generated by a linear acyclic causal model and at most one of the disturbances is Gaussian, independent component analysis (ICA) (Hyvärinen et al., 2001) can be exploited to discover the causal relations in a convenient way (Shimizu et al., 2006).

However, the above causal models seem too restrictive for real-life problems. If the assumed model is wrong, model-based causal discovery may give misleading results. Therefore, when the prior knowledge about the data model is not available, the assumed model should be general enough such that it could be adapted to approximate the true data generating process. On the other hand, the model should be identifiable such that it could distinguish causes from effects. In a large class of real-life problems, the following three effects usually exist. 1. The effect of the causes is usually nonlinear. 2. The final effect received by the target variable from all its causes contains some noise which is independent from the causes. 3. Sensors or measurements may introduce nonlinear distortions into the observed values of the variables. To address these issues, we propose a very realistic model, called post-nonlinear acyclic causal model with inner additive noise. In the two-variable case, we show the identifiability of this model under the assumption that the involved nonlinearities are invertible. We conjecture that this model is identifiable in very general situations, as illustrated by the experimental results.

## 2. Proposed Causal Model

Let us use a directed acyclic graph (DAG) to describe the generating process of the observed variables. We assume that each observed continuous variable  $x_i$ , corresponding to the  $i$ th node in the DAG, is generated by two stages. The first stage is a nonlinear transformation of its parents  $pa_i$ , denoted by  $f_{i,1}(pa_i)$ , plus some noise (or disturbance)  $e_i$  (which is independent from  $pa_i$ ). In the second stage, a nonlinear distortion  $f_{i,2}$  is applied to the output of the first stage to produce  $x_i$ . Mathematically, the generating process of  $x_i$  is

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

In this model, we assume that the nonlinearities  $f_{i,2}$  are continuous and invertible.  $f_{i,1}$  are not necessarily invertible. This model is very general, since it accounts for the nonlinear effect of the causes  $pa_i$  (by using  $f_{i,1}$ ), the noise effect in the transmission process from  $pa_i$  to  $x_i$  (using  $e_i$ ), and the nonlinear distortion caused by the sensor or measurement (using  $f_{i,2}$ ). In particular, in this paper we focus on the two-variable case. Suppose that  $x_2$  is caused by  $x_1$ . The relationship between  $x_1$  and  $x_2$  is then assumed to be

$$x_2 = f_{2,2}(f_{2,1}(x_1) + e_2), \quad (2)$$

where  $e_2$  is independent from  $x_1$ .

## 3. Identifiability<sup>1</sup>

### 3.1 Relation to post-nonlinear mixing ICA

We first consider the case where the nonlinear function  $f_{2,1}$  is also invertible. Let  $s_1 \triangleq f_{2,1}(x_1)$  and  $s_2 \triangleq e_2$ . As  $e_2$  is independent from  $x_1$ , obviously  $s_1$  is independent from  $s_2$ . The generating

1. When this paper was finalized, a systematic investigation of the identifiability of the proposed causal model was already reported in Zhang and Hyvärinen (2009), which contains some different results from this paper. Please refer to (Zhang and Hyvärinen, 2009) for more rigorous results on the identifiability.

process of  $(x_1, x_2)$ , given by Eq. 2, can be re-written as

$$\begin{cases} x_1 = f_{2,1}^{-1}(s_1), \\ x_2 = f_{2,2}(s_1 + s_2). \end{cases} \quad (3)$$

We can see that clearly  $x_1$  and  $x_2$  are post-nonlinear (PNL) mixtures of independent sources  $s_1$  and  $s_2$  (Taleb and Jutten, 1999). The PNL mixing model is a nice special case of the general nonlinear ICA model.

ICA is a statistical technique aiming to recover independent sources from their observed mixtures, without knowing the mixing procedure or any specific knowledge of the sources (Hyvärinen et al., 2001). The basic ICA model is linear ICA, in which the observed mixtures, as components of the vector  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ , are assumed to be generated from the independent sources  $s_1, s_2, \dots, s_n$ , with a linear transformation  $\mathbf{A}$ . Mathematically, we have  $\mathbf{x} = \mathbf{A}\mathbf{s}$ , where  $\mathbf{s} = (s_1, s_2, \dots, s_n)^T$ . Under weak conditions on the source distribution and the mixing matrix, ICA can recover the original independent sources up to the permutation and scaling indeterminacies with another transformation  $\mathbf{W}$ , by making the outputs as independent as possible. That is, the outputs of ICA, as components of  $\mathbf{y} = \mathbf{W}\mathbf{x}$ , produce an estimate of the original sources  $s_i$ . In the general nonlinear ICA problem,  $\mathbf{x}$  is assumed to be generated from independent sources  $s_i$  with an invertible nonlinear mapping  $\mathcal{F}$ , i.e.,  $\mathbf{x} = \mathcal{F}(\mathbf{s})$ , and the separation system is  $\mathbf{y} = \mathcal{G}(\mathbf{x})$ , where  $\mathcal{G}$  is another invertible nonlinear mapping. Generally speaking, nonlinear ICA is ill-posed: its solutions always exist but they are highly non-unique (Hyvärinen and Pajunen, 1999). To make the solution to nonlinear ICA meaningful, one usually needs to constrain the mixing mapping to have some specific forms (Jutten and Taleb, 2000).

The PNL mixing ICA model plays a nice trade-off of linear ICA and general nonlinear ICA. It is described as a linear transformation of the independent sources  $s_1, s_2, \dots, s_n$  with the transformation matrix  $\mathbf{A}$ , followed by a component-wise invertible nonlinear transformation  $\mathbf{f} = (f_1, f_2, \dots, f_n)^T$ . Mathematically,

$$x_i = f_i\left(\sum_{k=1}^n \mathbf{A}_{ik}s_k\right).$$

In matrix form, it is denoted as  $\mathbf{x} = \mathbf{f}(\mathbf{A}\mathbf{x})$ , where  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  and  $\mathbf{s} = (s_1, s_2, \dots, s_n)^T$ . In particular, from Eq. 3, one can see that for the causal model Eq. 2, the mixing matrix is  $\mathbf{A} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$ , and the post-nonlinearity is  $\mathbf{f} = (f_{2,1}^{-1}, f_{2,2})^T$ .

### 3.2 Identifiability of the Causal Model

The identifiability of the causal model Eq. 2 is then related to the separability of the PNL mixing ICA model. The PNL mixing model  $(\mathbf{A}, \mathbf{f})$  is said to be separable if the independent sources  $s_i$  could be recovered only up to some trivial indeterminacies (which includes the permutation, scaling, and mean indeterminacies) with a separation system  $(\mathbf{g}, \mathbf{W})$ . The output of the separation system is  $\mathbf{y} = \mathbf{W} \cdot \mathbf{g}(\mathbf{x})$ , where  $\mathbf{g}$  is a component-wise continuous and invertible nonlinear transformation. The separability of the PNL mixing model has been discussed in several contributions. As Achard and Jutten (2005) proved the separability under very general conditions, their result is briefly reviewed below.

**Theorem 1 (Separability of the PNL mixing model, by Achard & Jutten)** *Let  $(\mathbf{A}, \mathbf{f})$  be a PNL mixing system and  $(\mathbf{g}, \mathbf{W})$  the separation system. Let  $h_i \triangleq g_i \circ f_i$ . Assume the following conditions hold.*

- Each source  $s_i$  appears mixed at least once in the observations.

- $h_1, h_2, \dots, h_n$  are differentiable and invertible (same conditions as  $f_1, f_2, \dots, f_n$ ).
- There exists at most one Gaussian source.
- The joint density function of the sources  $s_i$  is differentiable, and its derivative is continuous on its support.

Then the output of the separation system  $(\mathbf{g}, \mathbf{W})$  has mutually independent components if and only if each  $h_i$  is linear and  $\mathbf{W}\mathbf{A}$  is a generalized permutation matrix.

The above theorem states that under the conditions stated above, by making the outputs of the separation system  $(\mathbf{g}, \mathbf{W})$  mutually independent, the original sources  $s_i$  and the mixing matrix  $\mathbf{A}$  could be uniquely estimated (up to some trivial indeterminacies). If  $f_{2,1}$  is invertible, the causal model Eq. 2, as a special case of the PNL mixing model, can then be identified. Thus, the theorem above implies the following proposition.

**Proposition 1 (Identifiability of the causal model with invertible nonlinearities)** *Suppose that  $x_1$  and  $x_2$  are generated according to the causal model Eq. 2 with both  $f_{2,2}$  and  $f_{2,1}$  differentiable and invertible. Further assume that at most one of  $f_{2,1}(x_1)$  and  $e_2$  is Gaussian, and that their joint density is differentiable, with the derivative continuous on its support. Then the causal relation between  $x_1$  and  $x_2$  can be uniquely identified.*

In the discussions above, we have constrained the nonlinearity  $f_{2,1}$  to be invertible. Otherwise,  $f_{2,1}^{-1}$  does not exist, and the causal model Eq. 2 is no longer a PNL mixing one. A rigorous proof of the identifiability of the causal model in this situation is under investigation. But it seems that it is identifiable under very general conditions, as verified by various experiments. It should be noted that when all the nonlinear functions  $f_{i,2}$  are constrained to be identity mappings, the proposed causal model is reduced to the nonlinear causal model with additive noise which was recently investigated by Hoyer et al. (2009). Interestingly, for this model, it was shown that in the two-variable case, the identifiability actually does not depend on the invertibility of the nonlinear function  $f_{2,1}$ .

## 4. Method for Identification

Given two variables  $x_1$  and  $x_2$ , we identify their causal relation by finding which one of the possible relations ( $x_1 \rightarrow x_2$  and  $x_2 \rightarrow x_1$ ) satisfies the assumed causal model. If the causal relation is  $x_1 \rightarrow x_2$  (i.e.,  $x_1$  and  $x_2$  satisfy the model Eq. 2), we can invert the data generating process Eq. 2 to recover the disturbance  $e_2$ , which is expected to be independent from  $x_1$ . One can then examine if a possible causal model is preferred in two steps: the first step is actually a constrained nonlinear ICA problem which aims to retrieve the disturbance corresponding to the assumed causal relation; in the second step we verify if the estimated disturbance is independent from the assumed cause using statistical tests.

### 4.1 A two-step method

Suppose the causal relation under examination is  $x_1 \rightarrow x_2$ . According to Eq. 2, if this causal relation holds, there exist nonlinear functions  $f_{2,2}^{-1}$  and  $f_{2,1}$  such that  $e_2 = f_{2,2}^{-1}(x_2) - f_{2,1}(x_1)$  is independent from  $x_1$ . Thus, we first perform nonlinear ICA using the structure in Figure 1. The outputs of this system are  $y_1 = x_1$ , and  $y_2 = g_2(x_2) - g_1(x_1)$ . In our experiments, we use multi-layer perceptrons (MLP's) to model the nonlinearities  $g_1$  and  $g_2$ . Parameters in  $g_1$  and  $g_2$  are learned by making  $y_1$  and  $y_2$  as independent as possible, which is achieved by minimizing the mutual information between  $y_1$  and  $y_2$ . The joint density of  $\mathbf{y} = (y_1, y_2)^T$  is  $p_{\mathbf{y}}(\mathbf{y}) = p_{\mathbf{x}}(\mathbf{x})/|\mathbf{J}|$ , where  $\mathbf{J}$  is the Jacobian matrix of the transformation from  $(x_1, x_2)$  to  $(y_1, y_2)$ ,

i.e.,  $\mathbf{J} = [\partial(y_1, y_2) / \partial(x_1, x_2)]$ . Clearly  $|\mathbf{J}| = |g'_2|$ . The joint entropy of  $\mathbf{y}$  is then

$$H(\mathbf{y}) = -E\{\log p_{\mathbf{y}}(\mathbf{y})\} = -E\{\log p_{\mathbf{x}}(\mathbf{x}) - \log |\mathbf{J}|\} = H(\mathbf{x}) + E\{\log |\mathbf{J}|\}.$$

Finally, the mutual information between  $y_1$  and  $y_2$  is

$$\begin{aligned} I(y_1, y_2) &= H(y_1) + H(y_2) - H(\mathbf{y}) \\ &= H(y_1) + H(y_2) - E\{\log |\mathbf{J}|\} - H(\mathbf{x}) \\ &= -E\{p_{y_1}(y_1)\} - E\{p_{y_2}(y_2)\} - E\{\log |g'_2|\} - H(\mathbf{x}), \end{aligned}$$

where  $H(\mathbf{x})$  does not depend on the parameters in  $g_1$  and  $g_2$  and can be considered as constant. One can easily find the gradient of  $I(y_1, y_2)$  w.r.t. the parameters in  $g_1$  and  $g_2$ , and minimize  $I(y_1, y_2)$  using gradient-descent methods. Details of the algorithm are skipped.

$y_1$  and  $y_2$  produced by the first step are the assumed cause and the estimated corresponding disturbance, respectively. In the second step, one needs to verify if they are independent, using statistical independence tests. We adopt the kernel-based statistical test (Gretton et al., 2008), with the significance level  $\alpha = 0.01$ . If  $y_1$  and  $y_2$  are not independent, indicating that  $x_1 \rightarrow x_2$  does not hold, we repeat the above procedure (with  $x_1$  and  $x_2$  exchanged) to verify if  $x_2 \rightarrow x_1$  holds. If  $y_1$  and  $y_2$  are independent, usually we can conclude that  $x_1$  causes  $x_2$ , and that  $g_1$  and  $g_2$  provide an estimate of  $f_{2,1}$  and  $f_{2,2}^{-1}$ , respectively. However, it is possible that both  $x_1 \rightarrow x_2$  and  $x_2 \rightarrow x_1$  hold, although the chance is very small. Therefore, for the sake of reliability, in this situation we also test if  $x_2 \rightarrow x_1$  holds. Finally, we can find the relationship between  $x_1$  and  $x_2$  among all four possible scenarios: 1.  $x_1 \rightarrow x_2$ , 2.  $x_2 \rightarrow x_1$ , 3. both causal relations are possible, and 4. there is no causal relation between  $x_1$  and  $x_2$  which follows our model.

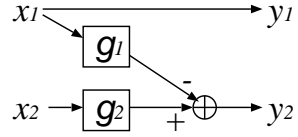


Figure 1: The constrained nonlinear ICA system used to verify if the causal relation  $x_1 \rightarrow x_2$  holds.

## 4.2 Practical considerations

The first issue that needs considering in practical implementation of our method is the model complexity, which is controlled by the number of hidden units in the MLP's modelling  $g_1$  and  $g_2$  in Figure 1. The system should have enough flexibility, and at the same time, to avoid overfitting, it should be as simple as possible. To this end, two ways are used. One is 10-fold cross-validation. The other is heuristic: we try different numbers of hidden units in a reasonable range (say, between 4 and 10); if the resulting causal relation does not change, we conclude that the result is feasible.

The second issue is the initialization of the nonlinearities  $g_1$  and  $g_2$  in Figure 1. If the nonlinear distortions  $f_{2,2}$  and  $f_{2,1}$  are very strong, it may take a long time for the nonlinear ICA algorithm in the first step to converge, and it is also possible that the algorithm converges to a local optimum. This can be avoided by using reasonable initializations for  $g_1$  and  $g_2$ . Two schemes are used in our experiments. One is motivated by visual inspection of the data distribution: we simply use a logarithm-like function to initialize  $g_1$  and  $g_2$  to make the transformed data more regular. The other is by making use of Gaussianization (Zhang and Chan, 2005). Roughly speaking, the central limit theorem states that sums of independent variables tend to be Gaussian. Since  $f_{2,2}^{-1}(x_2)$  in the causal model Eq. 2 is the sum of two independent variables, it is expected to be not very far from Gaussian. Therefore, for each variable which is very far from Gaussian, its associated nonlinearity ( $g_1$  or  $g_2$  in Figure 1) is initialized by the strictly

Data Set	#1	#2	#3	#4	#5	#6	#7	#8
Result	$x_1 \rightarrow x_2$	$x_1 \rightarrow x_2$	$x_1 \rightarrow x_2$	$x_1 \leftarrow^{\ddagger} x_2$	$x_1 \leftarrow x_2$	$x_1 \rightarrow x_2$	$x_1 \leftarrow x_2$	$x_1 \rightarrow x_2$

Table 1: Causal directions obtained. ( $\ddagger$  indicates that the causal relation is not significant.)

increasing function transforming this variable to standard Gaussian. In all experiments, these two schemes give the same final results.

## 5. Results

The proposed nonlinear causal discovery method has been applied to the “CauseEffectPairs” task proposed by Mooij et al. (2008) in the Pot-luck challenge. In this task, eight data sets are given; each of them contains the observed values of two variables  $x_1$  and  $x_2$ . The goal is to distinguish the cause from the effect for each data set. Figure 2 gives the scatterplots of  $x_1$  and  $x_2$  in all the eight data sets. Table 1 summaries our results. In particular, below we take data sets 1 and 8 as examples to illustrate the performance of our method.

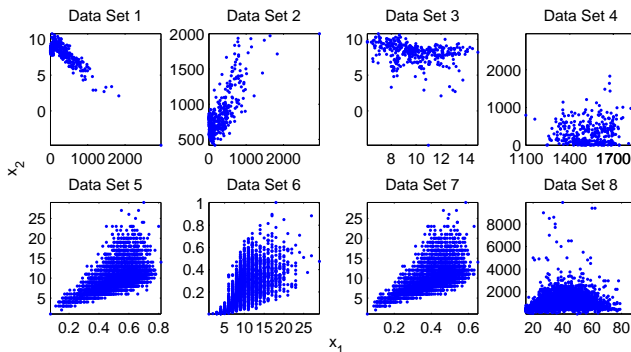


Figure 2: Scatterplot of  $x_1$  and  $x_2$  in each data set of the “CauseEffectPairs” task (Mooij et al., 2008).

The variable  $x_1$  in Data set 1 is non-negative and extremely non-Gaussian. We initialized the nonlinearity  $g_1$  with the transformation  $\log(2 + x_1)$  (Gaussianization was also tested and it finally produced the same causal relation). The scatterplot of  $y_1$  and  $y_2$  (as outputs of the constrained nonlinear ICA system in Figure 1) under each hypothesis ( $x_1 \rightarrow x_2$  or  $x_2 \rightarrow x_1$ ) is given in Figure 3(a,b). Clearly  $y_1$  and  $y_2$  are much more independent under hypothesis  $x_1 \rightarrow x_2$ . This is verified by the independence test results in the third row of Table 2. Note that a large test statistic tends to reject the null hypothesis (the independence between  $y_1$  and  $y_2$ ). Figure 4 shows the result on Data set 8. In this case, we applied the transformation  $\log(x_2 + 50)$  for initialization. By comparing (a) and (b) in Figure 4, also by inspecting the independence test results in the fourth row of Table 2, one can see clearly that  $x_1 \rightarrow x_2$ .

## 6. Conclusion

We proposed a very general nonlinear causal model for model-based causal discovery. This model takes into account the nonlinear effect of the causes, inner noise effect, and the sensor distortion, and is capable of approximating the data generating process of some real-life problems. We presented the identifiability of this model under the assumption that the involved nonlinearities are invertible. Experimental results illustrated that based on this model, one could

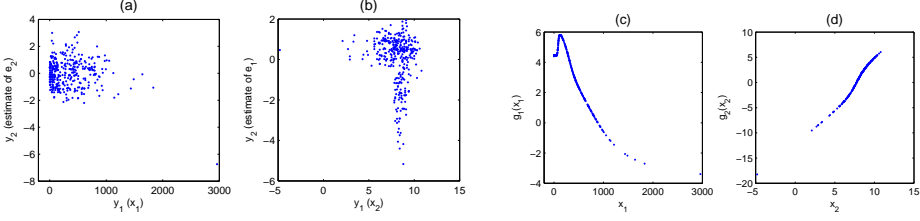


Figure 3: Result on Data set 1. (a)  $y_1$  vs.  $y_2$  under hypothesis  $x_1 \rightarrow x_2$ . (b) that under  $x_2 \rightarrow x_1$ . (c & d)  $x_1$  vs.  $g_1(x_1)$  and  $x_2$  vs.  $g_2(x_2)$  under hypothesis  $x_1 \rightarrow x_2$ .

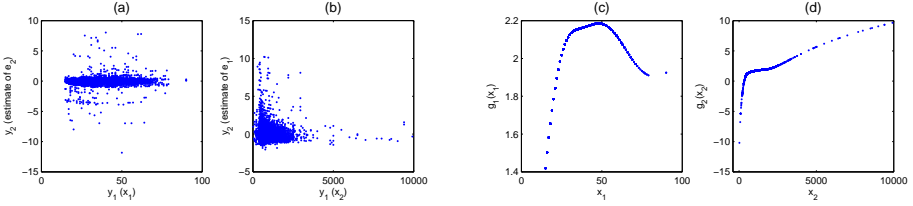


Figure 4: Result on Data set 8. For captions of the sub-figures, please refer to Figure 3.

Data Set	$x_1 \rightarrow x_2$ assumed		$x_2 \rightarrow x_1$ assumed	
	Threshold ( $\alpha = 0.01$ )	Statistic	Threshold ( $\alpha = 0.01$ )	Statistic
#1	$2.3 \times 10^{-3}$	$1.7 \times 10^{-3}$	$2.2 \times 10^{-3}$	$6.5 \times 10^{-3}$
#8	$1.2 \times 10^{-4}$	$1.2 \times 10^{-4}$	$1.1 \times 10^{-4}$	$7.4 \times 10^{-4}$

Table 2: Result of independence test on  $y_1$  and  $y_2$  for Data sets 1 and 8 under different assumed causal directions. For both data sets, the independence hypothesis is accepted in the scenario  $x_1 \rightarrow x_2$ , and rejected in the other scenario, with the significance level  $\alpha = 0.01$ .

successfully distinguish the cause from the effect, even if the nonlinear function of the cause is not invertible. An on-going work is to investigate the identifiability of this model under more general conditions.

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