Additive Noise Models: Identifiability Theorems, Learning Algorithms, Hidden Variables and Time Series

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Model Definition

We call the SCM, C, an addtive noise model if each observed variable X_j is associated with a node j in a directed acyclic graph G, and the value of X_j is obtained as a function of its parents in G, plus independent additive noise N_j, i.e.

$$X_j = f_j(\mathbf{PA}_j) + N_j \,, \qquad j = 1, \ldots, p \tag{1}$$

with jointly independent variables N_j. We will assume that the noise variables have strictly positive density.

Causal Minimality

For those models with strictly positive density, causal minimality reduces to the condition that each function f_j is not constant in any of its arguments.

Identifiability: The Bivariate Case

Hoyer et al. (2009) proves the following theorem about the identifiability of bivariate additive noise models.

Theorem

An additive noise model with two variables, i.e., $X_1 = N_1$ *and* $X_2 = f(X_1) + N_2$, *with* $N_1 \perp\!\!\!\perp N_2$, *is identifiable if it does not solve the following differential equation for all* x_i, x_j *with* $\nu''(x_j - f(x_i))f'(x_i) \neq 0$:

$$\xi''' = \xi'' \left(-\frac{\nu''' f'}{\nu''} + \frac{f''}{f'} \right) - 2\nu'' f'' f' + \nu' f''' + \frac{\nu' \nu''' f'' f'}{\nu''} - \frac{\nu' (f'')^2}{f'} ,$$

Here $\xi := \log p_{X_1}$ *and* $\nu := \log p_{N_2}$ *and we have skipped the arguments* $x_2 - f(x_1)$, x_1, *and* x_1 *for* ν, ξ, *and* f *and their derivatives, respectively.*

Corollary

Gaussian Noise: Assume that $\nu''' = \xi''' = 0$ everywhere. If a backward model exists, then f is linear.

Corollary

Assume that $f(x) = x$ and $p_x(x) = e^{-x-e^{-x}}$ and $p_n(n) = e^{-n-e^{-n}}$. With $p_y(y) = e^{-y-2\log(1+e^{y})}$, $\tilde{p}_n(\tilde{n}) = e^{-2\tilde{n}-e^{-\tilde{n}}}$ and $g(y) = \log(1 + e^{-y})$, one obtains:

$$p(x, y) = p_n(y - f(x))p_x(x) = \tilde{p}_n(x - g(y))p_y(y)$$

so the model is not identifiable.

Identifiability: From Bivariate to Multivariate

Definition

Consider an ANM with p variables. We call this SCM a *restricted additive noise model* if for all $j \in \mathbf{V}$, $i \in \mathbf{PA}_j$ and all sets $\mathbf{S} \subseteq \mathbf{V}$ with $\mathbf{PA}_j \setminus \{i\} \subseteq \mathbf{S} \subseteq \mathbf{ND}_j \setminus \{i, j\}$, there is an $x_\mathbf{S}$ with $p_\mathbf{S}(x_\mathbf{S}) > 0$, such that

$$\left(f_j(x_{\mathbf{PA}_j \setminus \{i\}}, X_i), P(X_i \,|\, X_\mathbf{S} = x_\mathbf{S}), P(N_j) \right)$$

satisfies the bivariate identifiability conditions.
We assume that the noise variables to have non-vanishing densities and the functions f_j are three times differentiable.

Identifiability: The Multivariate Case

Peters et al. (2014) proves a very interesting theorem. This theorem states how we can generalize a bivariate identifiability to the multivariate case, in this case ANM identifiability.

Theorem

Let $X_1, \ldots, X_p$ be generated by a restricted additive noise model with graph G_0 and assume that $P_{\mathbf{X}}$ satisfies causal minimality with respect to G_0, i.e., the functions f_j are not constant. Then, G_0 is identifiable from the joint distribution.

Identifiability: Post Non Linear (PNL) Models

Definition

PNL Models are introduced in Zhang and Hyvärinen (2009). A PNL is an SCM where each expresses each variable X_i as

$$X_i = g_i(f_i(\mathbf{PA}_i) + N_i), \quad i = 1, ..., n$$

Theorem (Bivariate Identifiability)

Assume that $x_2 = f_2(f_1(x_1) + e2)$ and $x_1 = g_2(g_1(x_2) + e1)$. *Densities and nonlinear functions are three times differentiable. We then have the following equation for every* (x_1, x_2) *satisfying* $\eta'' h' \neq 0$*:*

$$t_1 = g_2^{-1}(x_1),\ z_2 = f_2^{-1}(x_2),\ h = f_1 \circ g_2,\ h_1 = g_1 \circ f_2$$

$$\eta_1(t_1) = \log p_{t_1}(t_1) \ \ \eta_2(e_2) = \log p_{e_2}(e_2)$$

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

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

$$\frac{1}{h_1'} = \frac{\eta_1'' + \eta_2'' h'^2 - \eta_2' h''}{\eta_2'' h'}$$

	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	—

Figure: All unidentifiable cases with the assumptions made above

Learning Algorithms : Score Based Method

- The score proposed by Peters et al. (2014) and Nowzohour and Bühlmann (2016):

$$\hat{G} = \mathrm{argmin}_G \sum_{i=1}^{n} \mathrm{DM}(res_i^{G,\mathrm{RM}}, res_{-i}^{G,\mathrm{RM}}) + \lambda \#\mathrm{edges}$$

- DM = Dependence Method RM = Regression Method
- Idea : Noises are independent
- They do not prove (or even claim) that the minimizing of the above score is a consistent estimator for the correct DAG.
- Learning Algorithm: Greedy DAG Search or Brute Force (Only for small graphs)

Learning Algorithms : RESIT Algorithm

- First proposed in Peters et al. (2014)
- Assumption : Multivariate ANM + Causal Sufficiency
- Idea : $X_i \text{ is sink } \iff N_i \perp\!\!\!\perp \mathbf{X} \setminus \{X_i\}$
- The are two stages in the algorithm:
  - Stage 1 : Finding a causal order
  - Stage 2 : Estimating DAG by removing edges
- Number of Tests (Less than PC)
  - Stage 1 : $O(n^2)$
  - Stage 2 : $O(n)$

Learning Algorithms : RESIT Algorithm

Algorithm 1 Regression with subsequent independence test (RESIT)

Input: I.i.d. samples of a p-dimensional distribution on $(X_1, \ldots, X_p)$
$S := \{1, \ldots, p\}, \pi := [\,]$
PHASE 1: Determine topological order.
repeat
    for $k \in S$ **do**
        Regress X_k on $\{X_i\}_{i \in S \setminus \{k\}}$.
        Measure dependence between residuals and $\{X_i\}_{i \in S \setminus \{k\}}$.
    end for
    Let k^* be the k with the weakest dependence.
    $S := S \setminus \{k^*\}$
    $\mathrm{pa}(k^*) := S$
    $\pi := [k^*, \pi]$ (π will be the topological order, its last component being a sink)
until $\#S = 0$
PHASE 2: Remove superfluous edges.
for $k \in \{2, \ldots, p\}$ **do**
    for $\ell \in \mathrm{pa}(\pi(k))$ **do**
        Regress $X_{\pi(k)}$ on $\{X_i\}_{i \in \mathrm{pa}(\pi(k)) \setminus \{\ell\}}$.
        if residuals are independent of $\{X_i\}_{i \in \{\pi(1), \ldots, \pi(k-1)\}}$ **then**
            $\mathrm{pa}(\pi(k)) := \mathrm{pa}(\pi(k)) \setminus \{\ell\}$
        end if
    end for
end for
Output: $(\mathrm{pa}(1), \ldots, \mathrm{pa}(p))$

RESIT Algorithm : Performance (Linear Setting)

$\beta_{jk} \sim [-2, -0.1] \cup [0.1, 2]$ $\quad N_j \sim K_j \cdot \mathrm{sign}(M_j) \cdot |M_j|^{\alpha_j}$ such that $M_j \sim N(0, 1)$, $K_j \sim U(0.1, 0.5)$ and $\alpha_j \sim U([2, 4])$.

	GDS	BF	RESIT	LiNGAM	PC	CPC	GES	RAND
				$p = 4, n = 100$				
DAG	0.7 ± 0.9	0.6 ± 0.8	1.2 ± 1.3	1.9 ± 1.2	3.5 ± 1.5	3.6 ± 1.4	3.1 ± 1.7	4.4 ± 1.0
CPDAG	1.1 ± 1.5	0.9 ± 1.4	1.5 ± 1.7	2.4 ± 1.5	2.4 ± 1.7	2.3 ± 1.6	2.0 ± 2.0	4.3 ± 1.4
				$p = 4, n = 500$				
DAG	0.2 ± 0.6	0.1 ± 0.3	0.6 ± 0.8	0.5 ± 0.8	3.1 ± 1.4	3.2 ± 1.4	2.9 ± 1.6	4.1 ± 1.2
CPDAG	0.3 ± 0.9	0.2 ± 0.5	0.9 ± 1.3	0.8 ± 1.2	1.9 ± 1.8	1.6 ± 1.7	1.6 ± 1.9	3.9 ± 1.4
				$p = 15, n = 100$				
DAG	12.2 ± 5.3	–	25.2 ± 8.3	11.1 ± 3.7	13.0 ± 3.6	13.7 ± 3.7	12.7 ± 4.2	57.4 ± 26.4
CPDAG	13.2 ± 5.4	–	27.0 ± 8.5	12.4 ± 3.9	10.7 ± 3.5	10.8 ± 3.8	12.4 ± 4.9	58.5 ± 27.1
				$p = 15, n = 500$				
DAG	6.1 ± 6.4	–	51.2 ± 17.8	3.4 ± 2.8	10.2 ± 3.8	10.8 ± 4.2	8.7 ± 4.6	57.6 ± 24.2
CPDAG	6.8 ± 6.9	–	54.5 ± 18.5	4.5 ± 3.8	8.2 ± 4.6	7.5 ± 4.4	7.1 ± 5.6	58.9 ± 25.0

Figure: Structural Hamming Distance of Estimated Graph

RESIT Algorithm : Performance (Non Linear Setting)

Functions sampled from a Gaussian process with $BW = 1$. Gaussian Noise with random variance.

	GDS	BF	RESIT	LiNGAM	PC	CPC	GES	RAND
	$p = 4, n = 100$							
DAG	1.5 ± 1.4	1.0 ± 1.0	1.7 ± 1.3	3.5 ± 1.2	3.5 ± 1.5	3.8 ± 1.4	3.5 ± 1.3	4.0 ± 1.3
CPDAG	1.7 ± 1.7	1.2 ± 1.4	2.0 ± 1.6	3.0 ± 1.4	2.9 ± 1.5	2.7 ± 1.4	3.4 ± 1.7	3.9 ± 1.4
	$p = 4, n = 500$							
DAG	0.5 ± 0.9	0.3 ± 0.5	0.8 ± 0.9	3.7 ± 1.2	3.5 ± 1.5	3.8 ± 1.5	3.3 ± 1.5	4.1 ± 1.2
CPDAG	0.6 ± 1.1	0.6 ± 1.0	1.0 ± 1.3	3.0 ± 1.7	3.1 ± 1.9	2.8 ± 1.8	3.4 ± 1.9	3.8 ± 1.6
	$p = 15, n = 100$							
DAG	14.3 ± 4.9	–	15.4 ± 5.7	15.4 ± 3.6	14.2 ± 3.5	15.5 ± 3.6	24.8 ± 6.3	56.8 ± 24.1
CPDAG	15.1 ± 5.4	–	16.5 ± 5.9	15.3 ± 4.0	13.3 ± 3.6	13.3 ± 4.0	26.4 ± 6.5	58.0 ± 24.7
	$p = 15, n = 500$							
DAG	13.0 ± 8.4	–	10.1 ± 5.7	21.4 ± 6.9	13.9 ± 4.5	15.1 ± 4.8	26.8 ± 8.5	56.1 ± 26.8
CPDAG	14.2 ± 9.2	–	11.3 ± 6.3	21.1 ± 7.3	13.7 ± 4.9	13.4 ± 5.1	28.6 ± 8.8	57.0 ± 27.3

Figure: Structural Hamming Distance of Estimated Graph

Real Dataset?

Average Temperature, Altitude, Duration of Sunlight from 349 German weather stations.

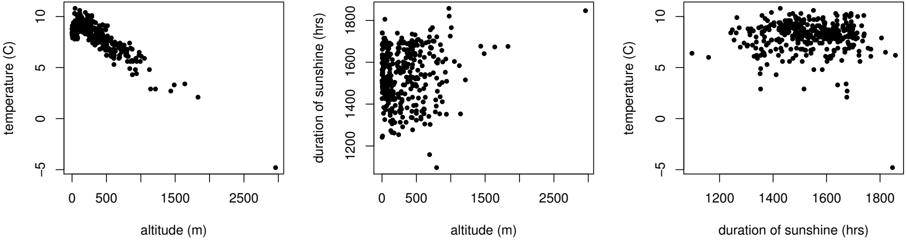


Figure: Scatter plot of the data

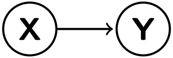
Real Dataset!

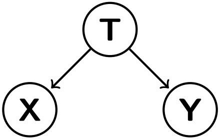
Output graph of different algorithms:

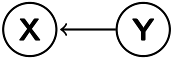
Method	Graph
LiNGAM	$T \rightarrow A$
PC	$T \rightarrow A \leftarrow DS$
CPC	$T \rightarrow A \leftarrow DS$
GDS	$T \leftarrow A \rightarrow DS$
BF	$T \leftarrow A \rightarrow DS$
RESIT	$T \leftarrow A \rightarrow DS$

Confounder Detection in The Bivariate Case

$$\begin{cases} X = f(T) + N_X \\ Y = g(T) + N_Y \end{cases}$$



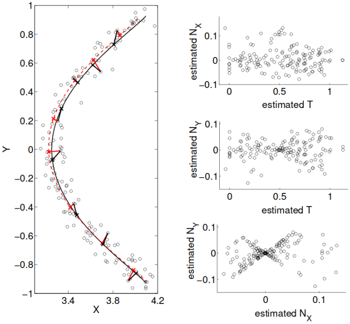




Naive Method: Dimension Reduction

$$\hat{T}_k = \text{argmin}_{t\in[0,1]} ||(X_k, Y_k) - \mathbf{s}(t)||_2$$

find $\hat{\mathbf{s}}$ that minimizes $\sum_{k=1}^{n} ||(X_k, Y_k) - \mathbf{s}(\hat{T}_k)||_2$. Then test the independence of noise variables



Confounder: ICAN Algorithm

Algorithm 1 Identifying Confounders using Additive Noise Models (ICAN)

Input: $(X_1, Y_1), \ldots, (X_n, Y_n)$ (normalized)

Initialization:
Fit a curve $\hat{\mathbf{s}}$ to the data that minimizes ℓ_2 distance: $\hat{\mathbf{s}} := \operatorname{argmin}_{\mathbf{s} \in \mathcal{S}} \sum_{k=1}^{n} \operatorname{dist}\big(\mathbf{s}, (X_k, Y_k)\big)$.

repeat
  Projection:
  $\hat{T} := \operatorname{argmin}_T \operatorname{DEP}(\hat{N}_X, \hat{N}_Y) + \operatorname{DEP}(\hat{N}_X, T) + \operatorname{DEP}(\hat{N}_Y, T)$ with $(\hat{N}_{X,k}, \hat{N}_{Y,k}) = (X_k, Y_k) - \hat{\mathbf{s}}(T_k)$
  if $\hat{N}_X \perp\!\!\!\perp \hat{N}_Y$ and $\hat{N}_X \perp\!\!\!\perp \hat{T}$ and $\hat{N}_Y \perp\!\!\!\perp \hat{T}$ **then**
    Output: $(\hat{T}_1, \ldots, \hat{T}_n)$, $\hat{u} = \hat{\mathbf{s}}_1$, $\hat{v} = \hat{\mathbf{s}}_2$, and $\frac{\mathbb{V}\mathrm{ar}\,\hat{N}_X}{\mathbb{V}\mathrm{ar}\,\hat{N}_Y}$.
    Break.
  end if
  Regression:
  Estimate $\hat{\mathbf{s}}$ by regression $(X, Y) = \hat{\mathbf{s}}(\hat{T}) + \hat{\mathbf{N}}$. Set $\hat{u} = \hat{\mathbf{s}}_1, \hat{v} = \hat{\mathbf{s}}_2$.
until K iterations

Output: Data cannot be fitted by a CAN model.

- The Naive method does not work even in simple cases.
- ICAN was first introduced in Janzing et al. (2009).
- Idea: Minimizing dependence instead of the l_2 norm.
- Proof of consistency only for the low noise regime. The algorithm seems to work in large noise regime as well.

Time Series : TiMINo

Definition

Consider a time series $\mathbf{X}_t = (X_t^i)_{i \in V}$. We say the time series satisfies a *TiMINo* if there is a $p > 0$ and if $\forall i \in V$ there are sets $\mathbf{PA}_0^i \subseteq X^{V \setminus \{i\}}, \mathbf{PA}_k^i \subseteq X^V$, s.t. $\forall t$

$$X_t^i = f_i\big((\mathbf{PA}_p^i)_{t-p}, \ldots, (\mathbf{PA}_1^i)_{t-1}, (\mathbf{PA}_0^i)_t, N_t^i\big)\ , \qquad (2)$$

with N_t^i (jointly) independent and for each i, N_t^i identically distributed in t and the full time graph is acyclic.

Peters et al. (2013)

Time Series : TiMINo

Algorithm 1 TiMINo causality

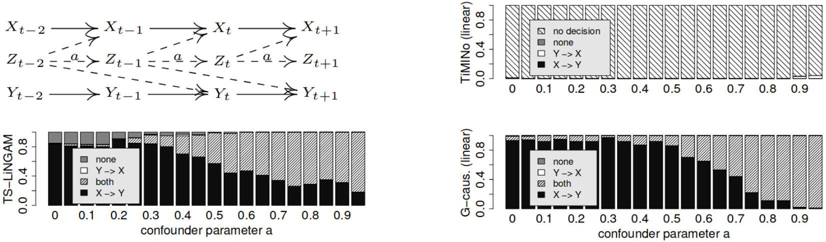
Input: Samples from a d-dimensional time series of length T: $(\mathbf{X}_1, \ldots, \mathbf{X}_T)$, maximal order p
$S := (1, \ldots, d)$
repeat
  for k in S **do**
    Fit TiMINo for X_t^k using $X_{t-p}^k, \ldots, X_{t-1}^k, X_{t-p}^i, \ldots, X_{t-1}^i, X_t^i$ for $i \in S \setminus \{k\}$
    Test if residuals are indep. of $X^i, i \in S$.
  end for
  Choose k^* to be the k with the weakest dependence. (If there is no k with independence, break and output: "I do not know - bad model fit").
  $S := S \setminus \{k^*\}; \quad \mathrm{pa}(k^*) := S$
until length(S)= 1
For all k remove all parents that are not required to obtain independent residuals.
Output: $(\mathrm{pa}(1), \ldots, \mathrm{pa(d)})$

TiMINo causality has to be provided with a fitting method. e.g. VAR fitting, generalized additive models (gam) and GP regression.

Time Series : Granger Causality vs. TiMINo

- TiMINo allows instantaneous effects.
- Shifted Time Series $(\tilde{X}_t^i = X_{t-l_i}^i)$ for example in fMRI Data. There might be causal relations backwards in time and Granger Causality might fail in these cases. In TiMINo, the summary graph is identifiable.
- in some cases, TiMINo output is "Can't Decide"

- a simple case with confounder:



- $$\begin{cases} X_t &= 0.8X_{t-1} + 0.3N_{X,t} \\ Y_t &= 0.4Y_{t-1} + (X_{t-1} - 1)^2 + 0.3N_{Y,t} \\ Z_t &= 0.4Z_{t-1} + 0.5\cos(Y_{t-1}) + \sin(Y_{t-1}) + 0.3N_{Z,t} \end{cases}$$

DAG	$\text{Granger}_{\text{lin}}$	$\text{Granger}_{\text{nonlin}}$	$\text{TiMINo}_{\text{lin}}$	$\text{TiMINo}_{\text{gam}}$	$\text{TiMINo}_{\text{GP}}$	TS-LiNGAM
correct	69%	0%	0%	95%	94%	12%
wrong	31%	100%	0%	1%	1%	88%
no dec.	0%	0%	100%	4%	5%	0%

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