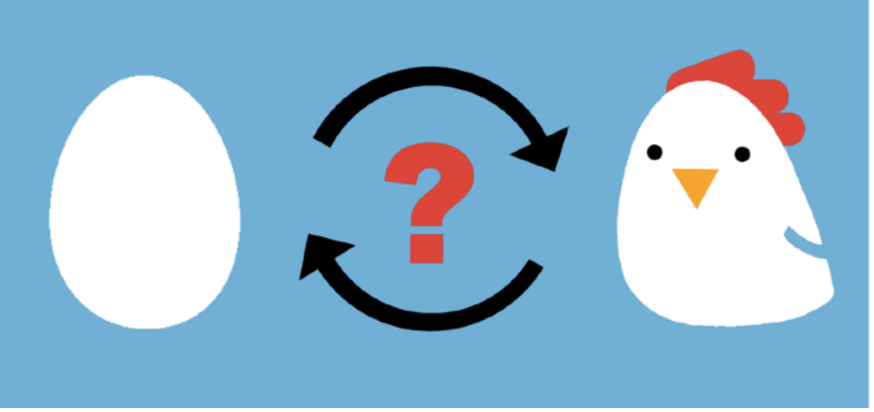


Causality and Machine Learning *(80-816/516)*

Classes 11 & 12 (Feb 18 & 20, 2025)

Linear, Non-Gaussian Causal Models for Causal Discovery (After 2005)

Instructor:

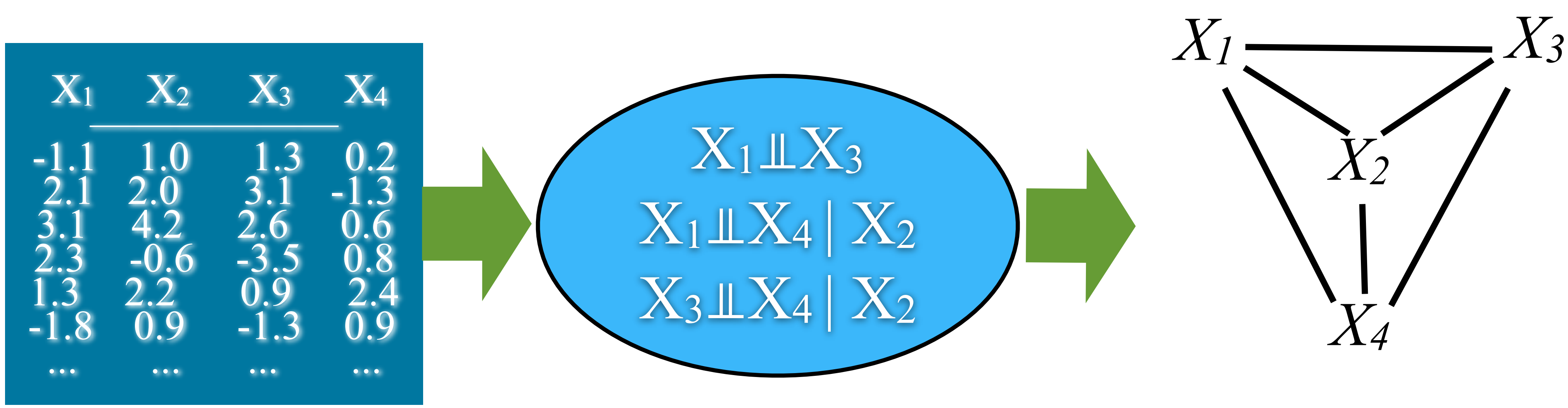
Kun Zhang (kunz1@cmu.edu)

Zoom link: https://cmu.zoom.us/j/8214572323)

Office Hours: W 3:00–4:00PM (on Zoom or in person); other times by appointment

PC Assumes No Confounder

- Make use of conditional independence constraints
- Rely on causal Markov condition + faithfulness assumption
- Output represented by a pattern (CPDAG)



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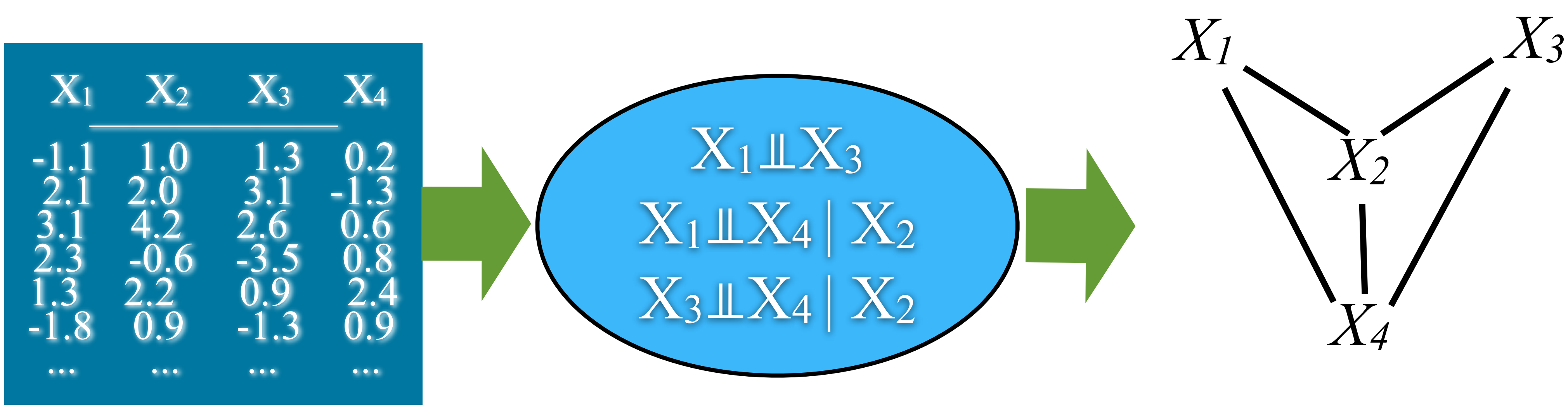

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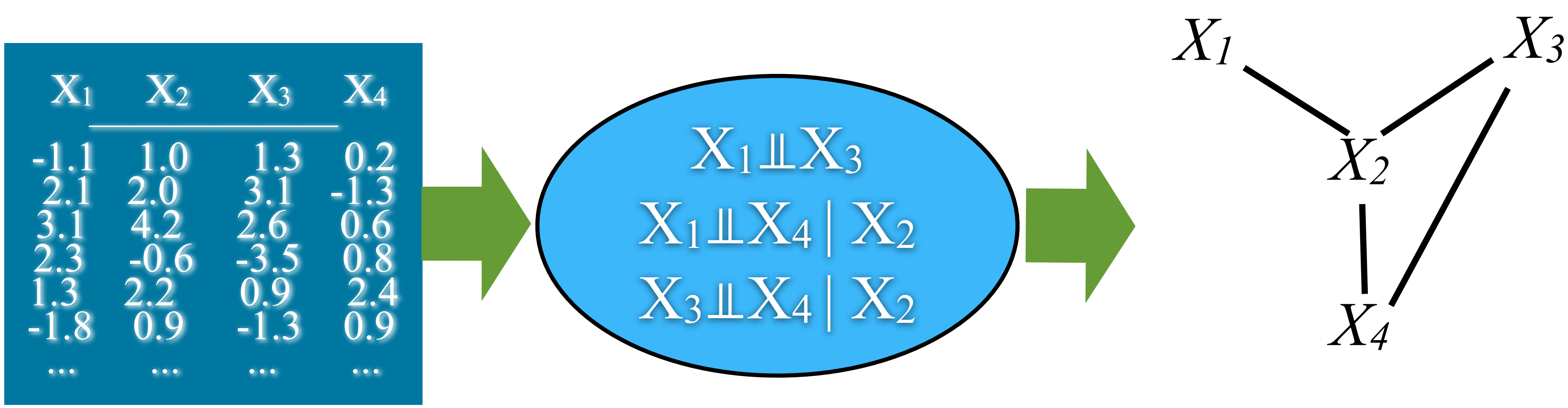

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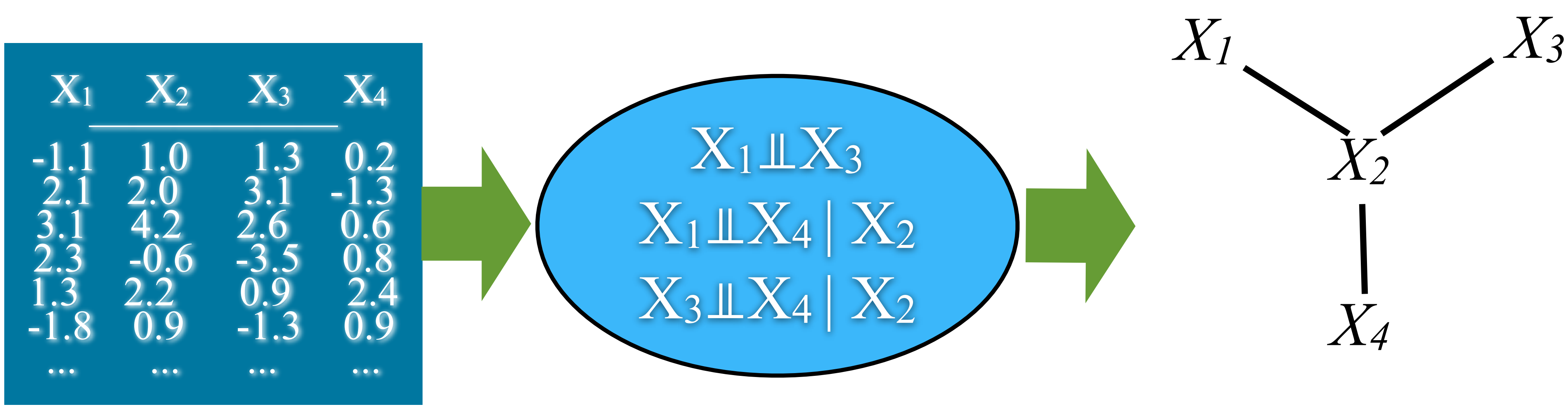

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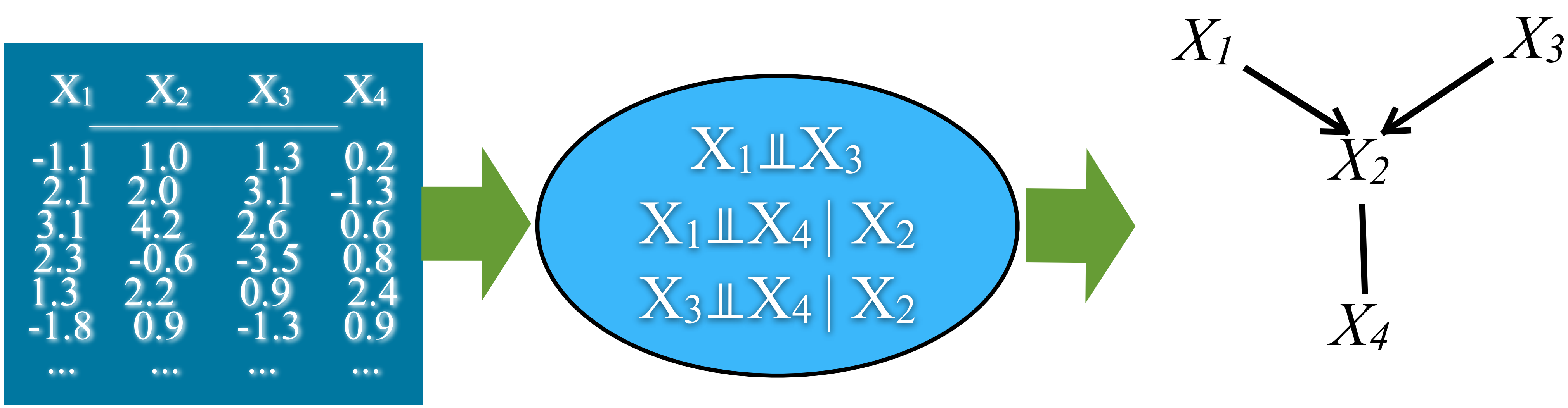

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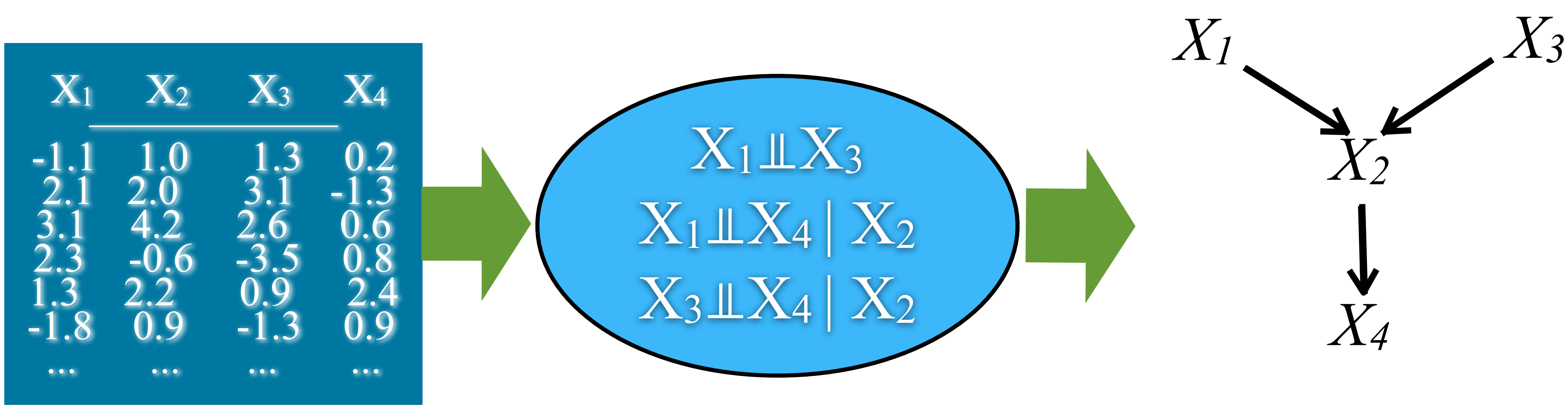

FCI Allows Confounders

Example I

$X_1 \perp\!\!\!\perp X_2;$

$X_1 \perp\!\!\!\perp X_4 \mid X_3;$

$X_2 \perp\!\!\!\perp X_4 \mid X_3.$

FCI Allows Confounders

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$X_1 \perp\!\!\!\perp X_2;$

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Possible to have confounders behind X_3 and X_4?

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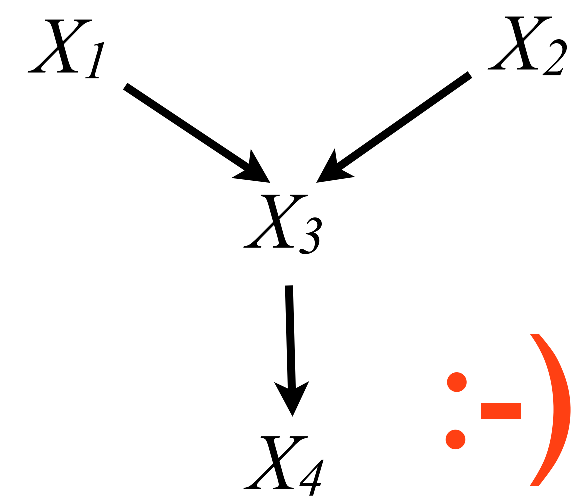

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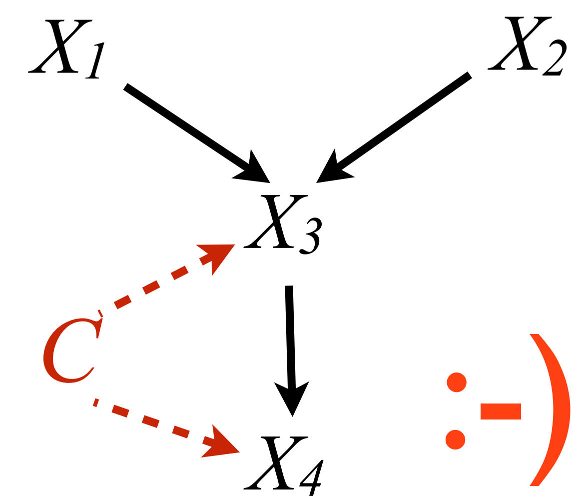

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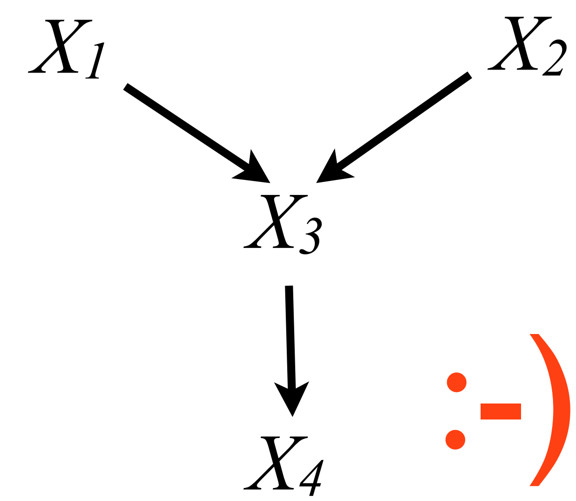

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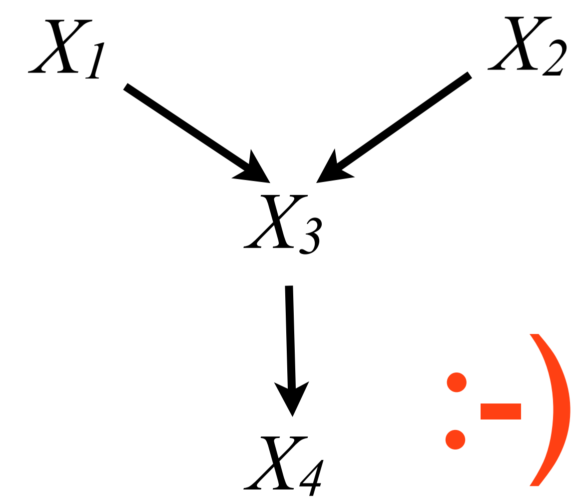

E.g., X_1: Raining; X_3: wet ground; X_4: slippery.

FCI Allows Confounders

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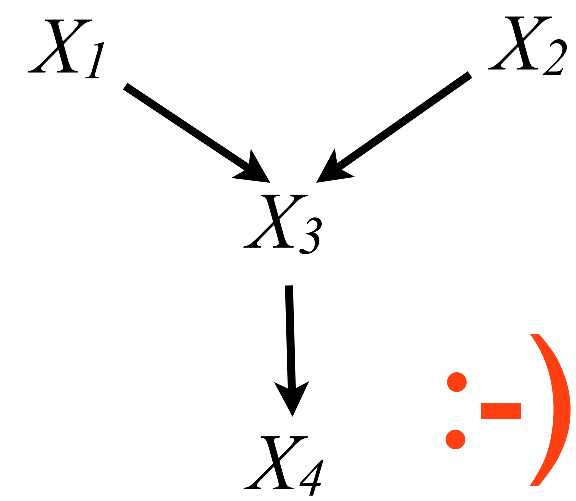

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Example II

$X_1 \perp\!\!\!\perp X_3;$

$X_1 \perp\!\!\!\perp X_4;$

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FCI Allows Confounders

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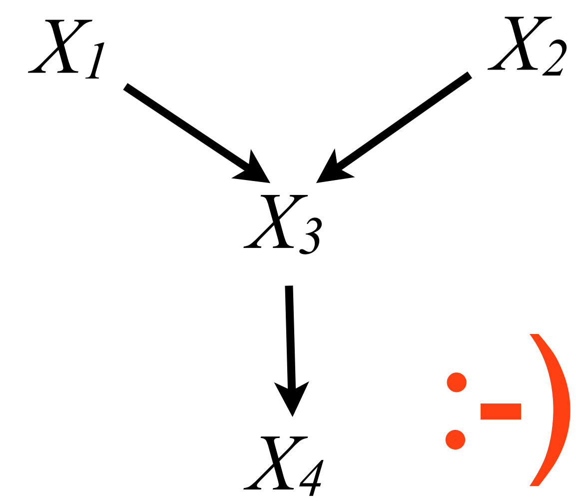

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Example II

$X_1 \perp\!\!\!\perp X_3;$

$X_1 \perp\!\!\!\perp X_4;$

$X_2 \perp\!\!\!\perp X_3.$

Are there confounders behind X_2 and X_4?

FCI Allows Confounders

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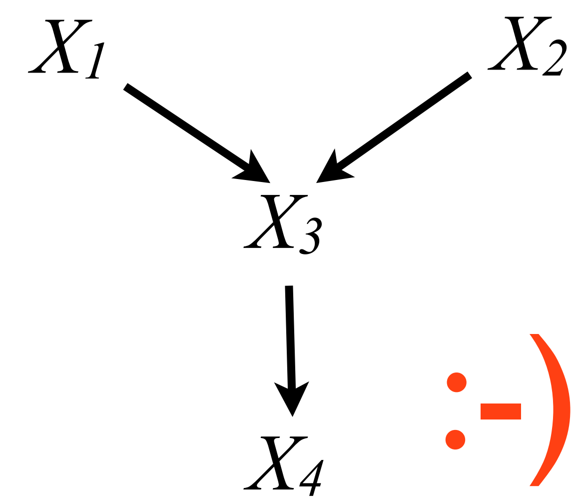

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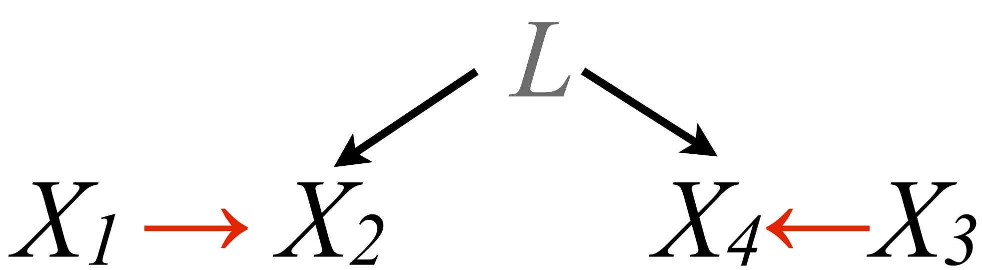

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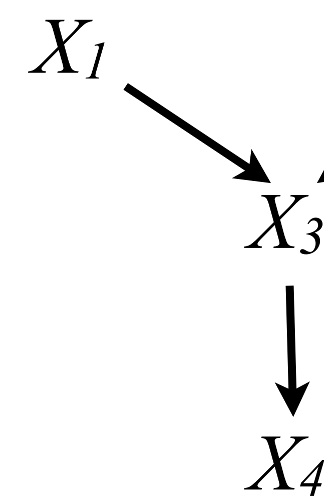

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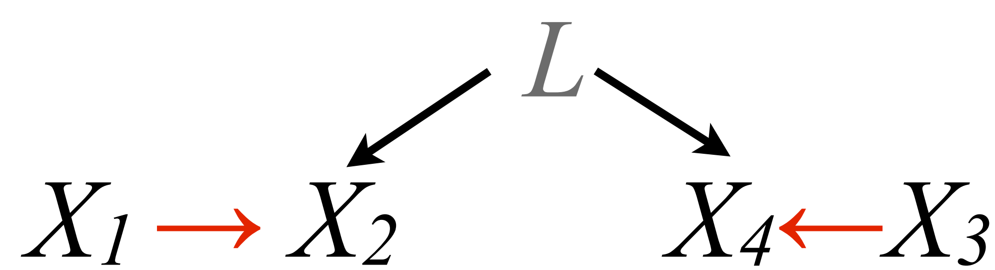
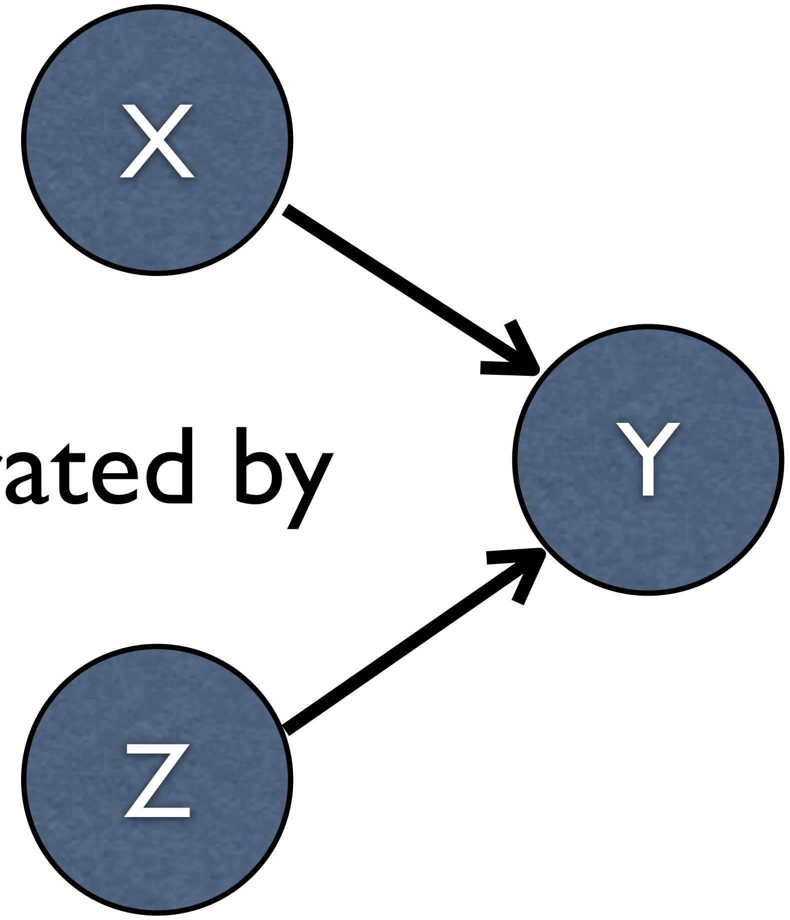


E.g., X_1: I am not sick; X_2: I am in this lecture room; X_4: you are in this lecture room; X_3: you are not sick.

GES Assumes No Confounder

Suppose data were generated by



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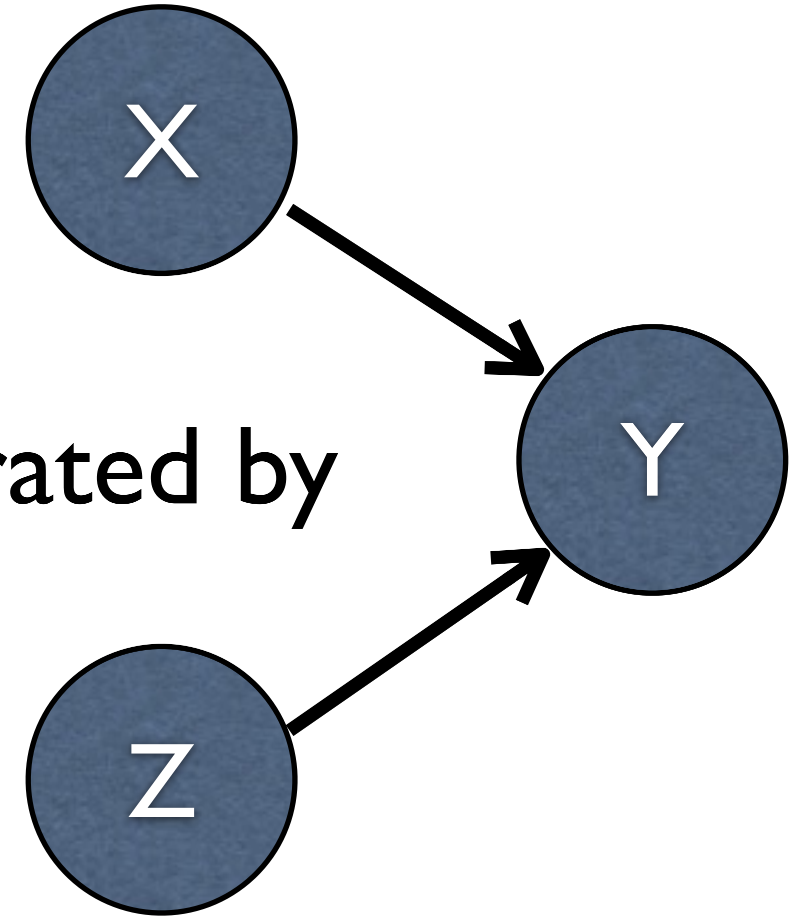
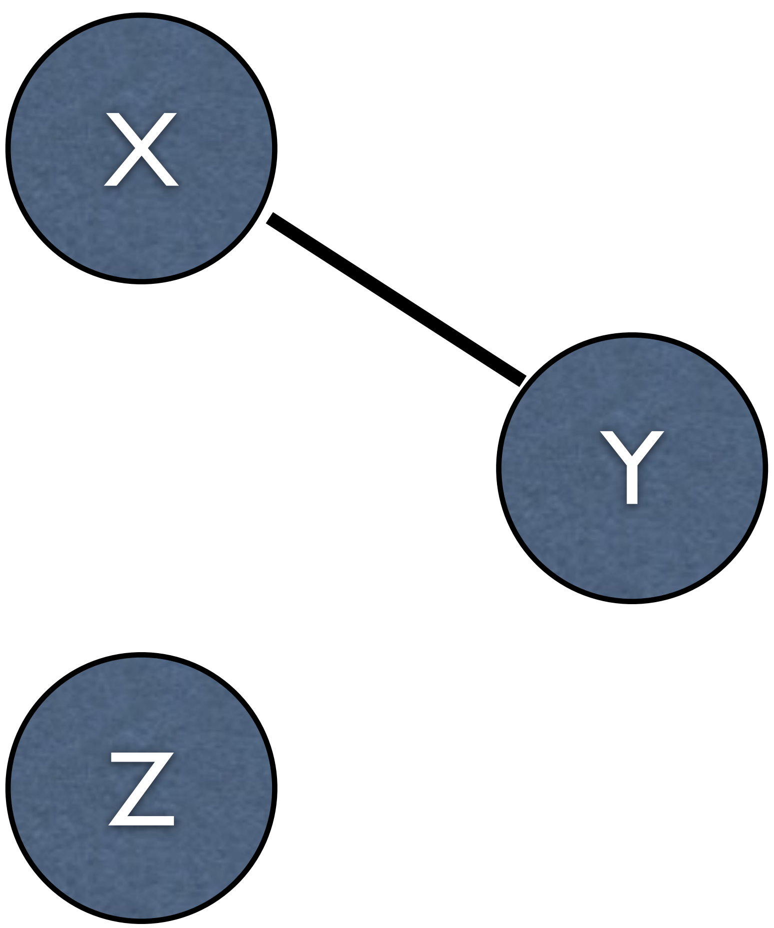


(1)



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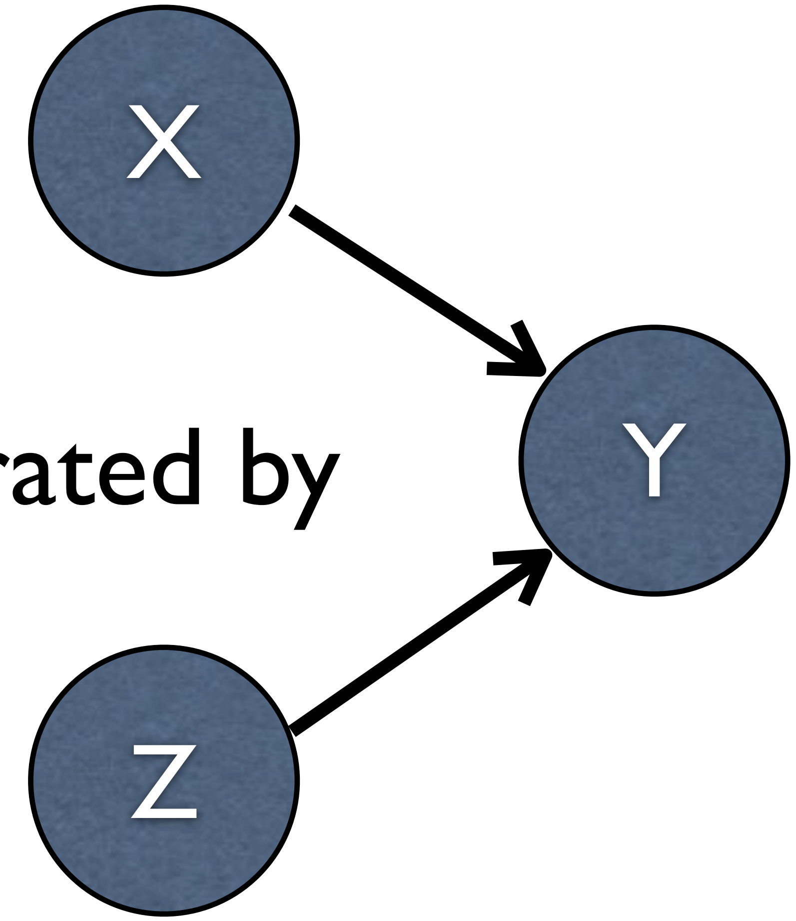

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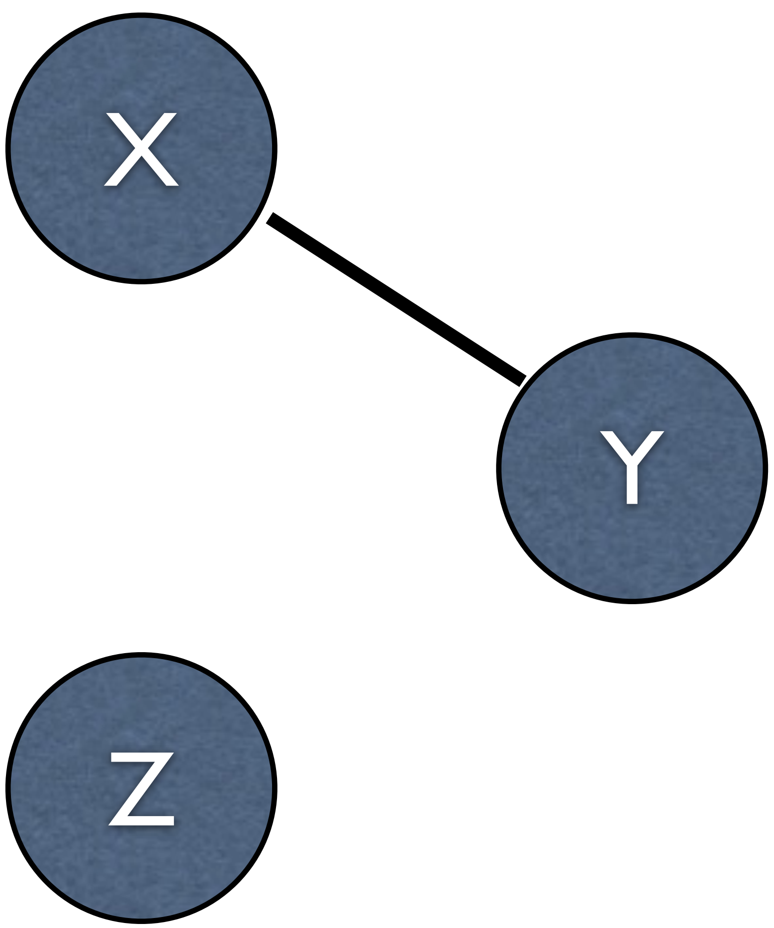
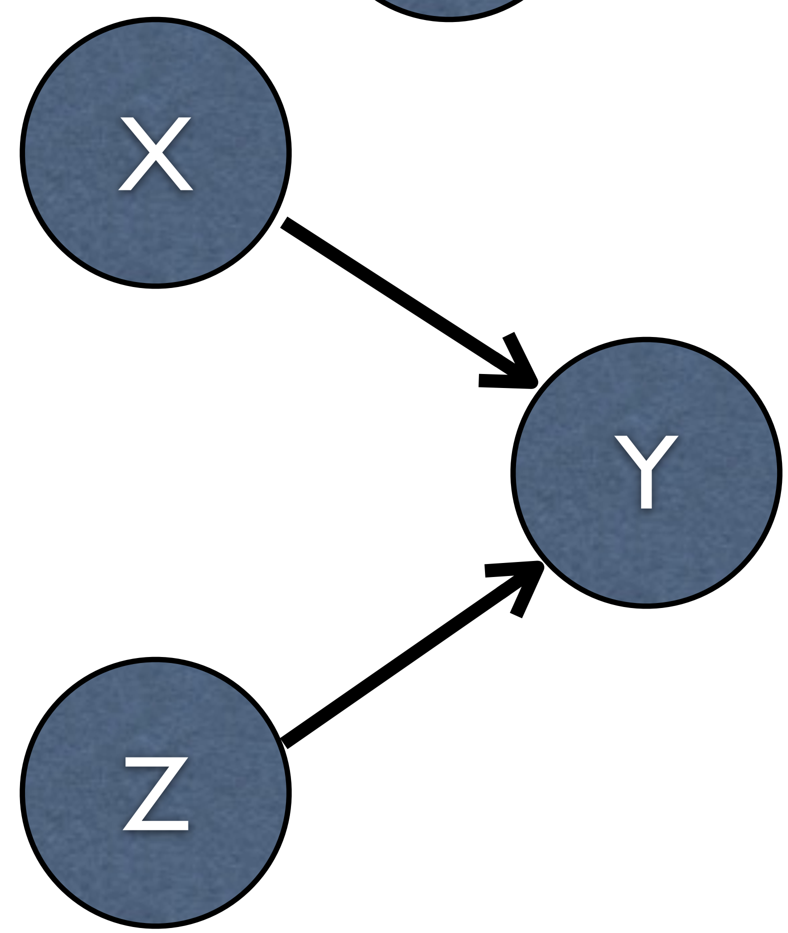
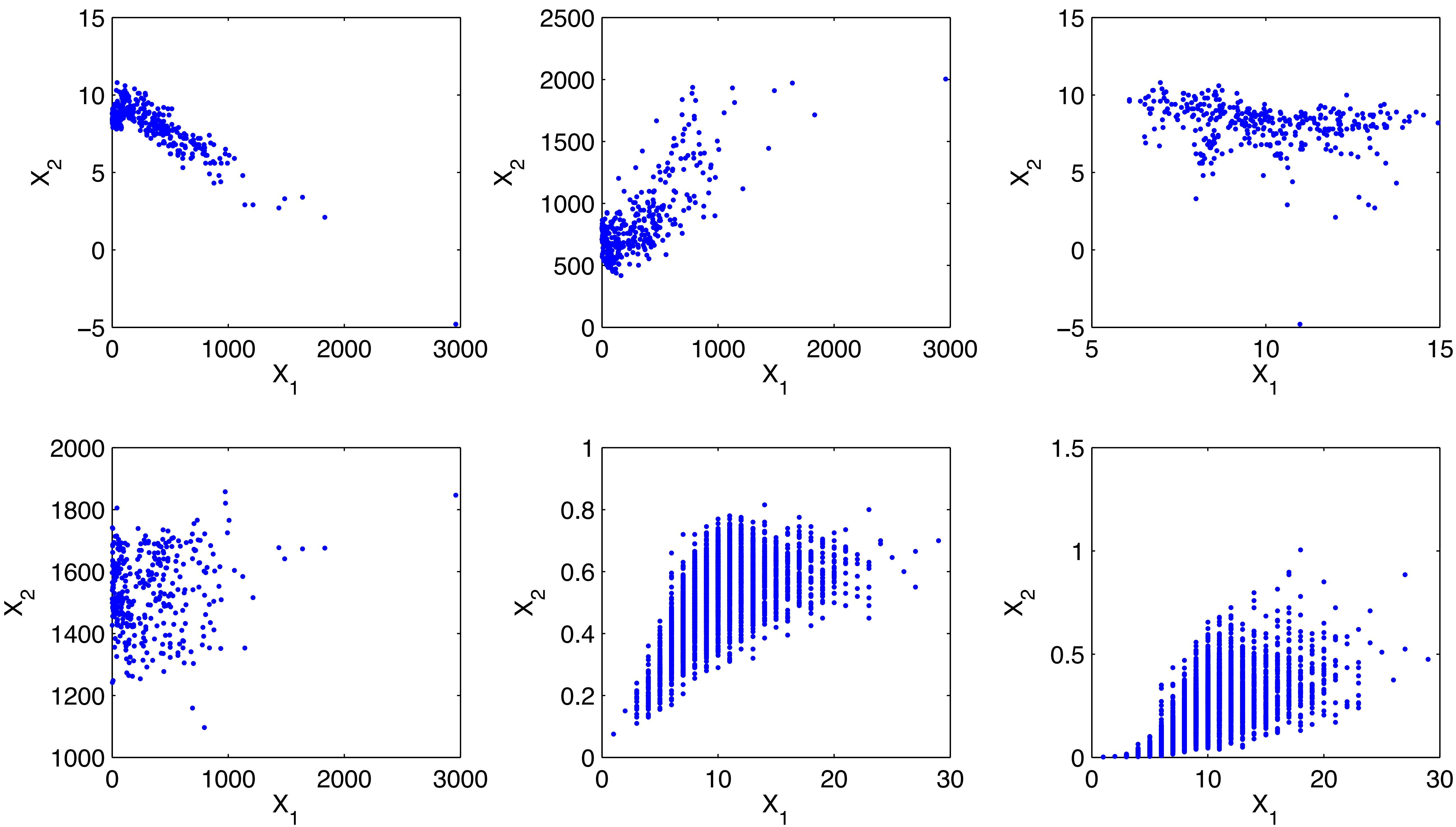


(2)



Distinguishing Cause from Effect:
Examples (Tübingen Cause-Effect Pairs)

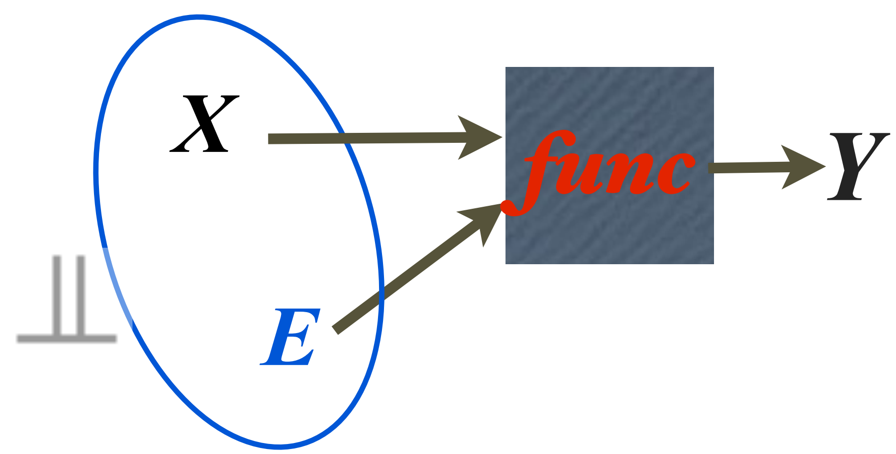


A Causal Process

rain $\longrightarrow$ *wet ground*

A Causal Process

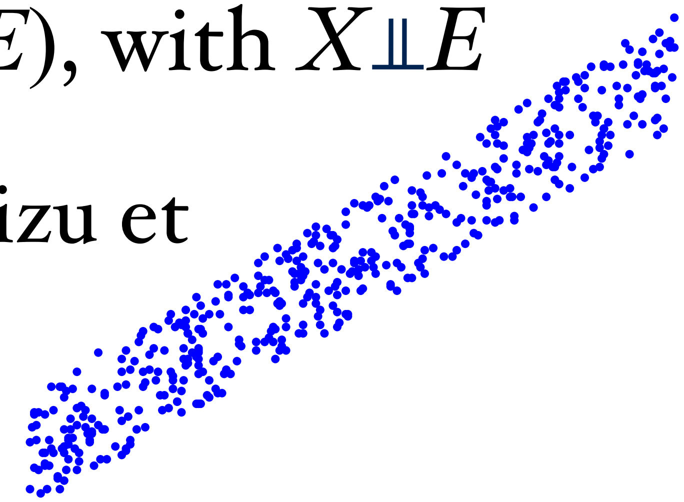
rain ⟶ *wet ground*



Functional Causal Model

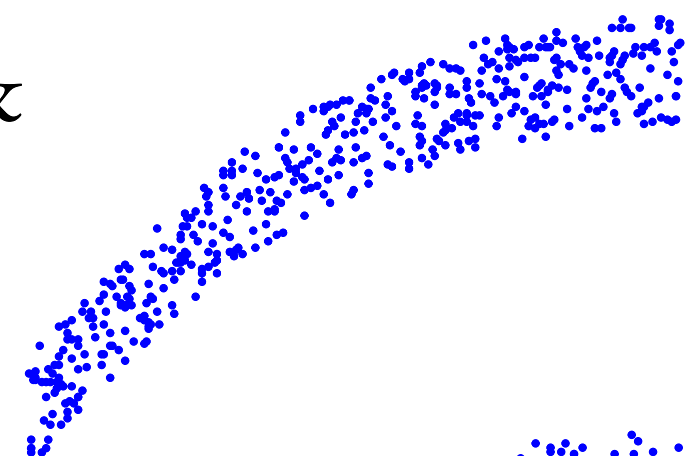
- A **functional causal model** represents effect as a function of direct causes and noise: $Y = f(X, E)$, with $X \perp\!\!\!\perp E$
- Linear non-Gaussian acyclic causal model (Shimizu et al., '06)

$$Y = a \cdot X + E$$



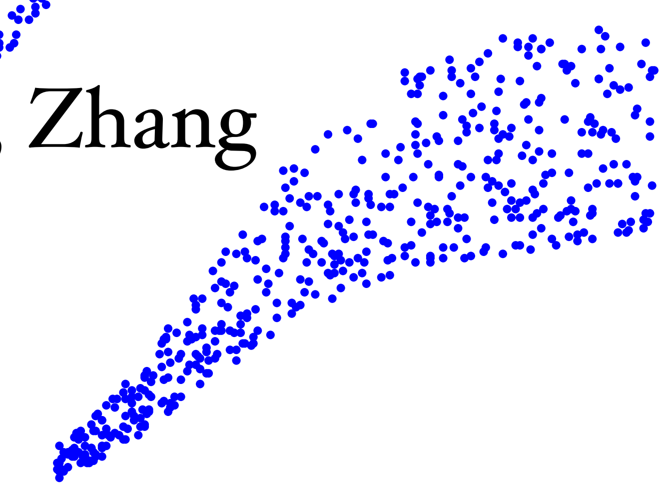
- Additive noise model (Hoyer et al., '09; Zhang & Hyvärinen, '09b)

$$Y = f(X) + E$$

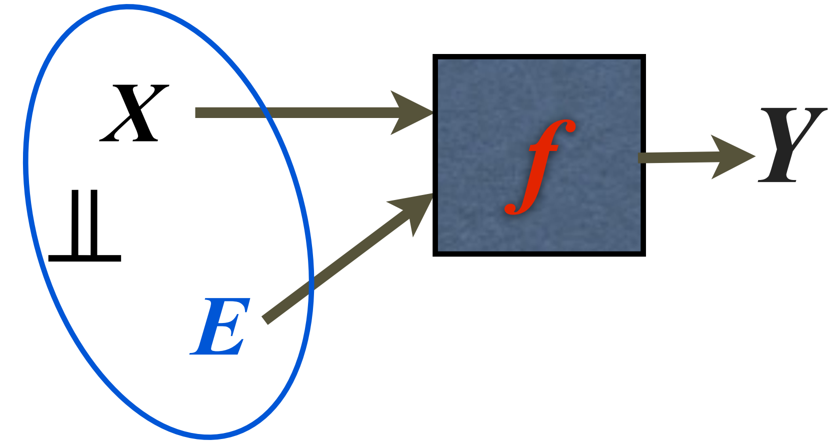


- Post-nonlinear causal model (Zhang & Chan, '06; Zhang & Hyvärinen, '09a)

$$Y = f_2\,(\,f_1(X) + E\,)$$



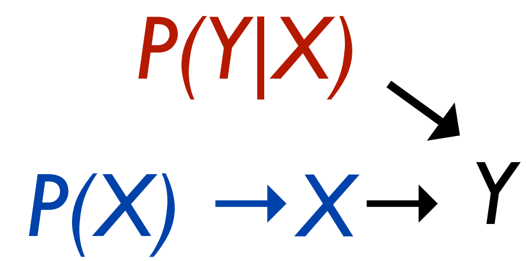
Functional Causal Models



- Effect generated from cause with **independent noise** (Pearl et al.):

$$Y = f(X, E)$$

  - A way to encode the intuition "the generating process for X is 'independent' from that generates Y from X"

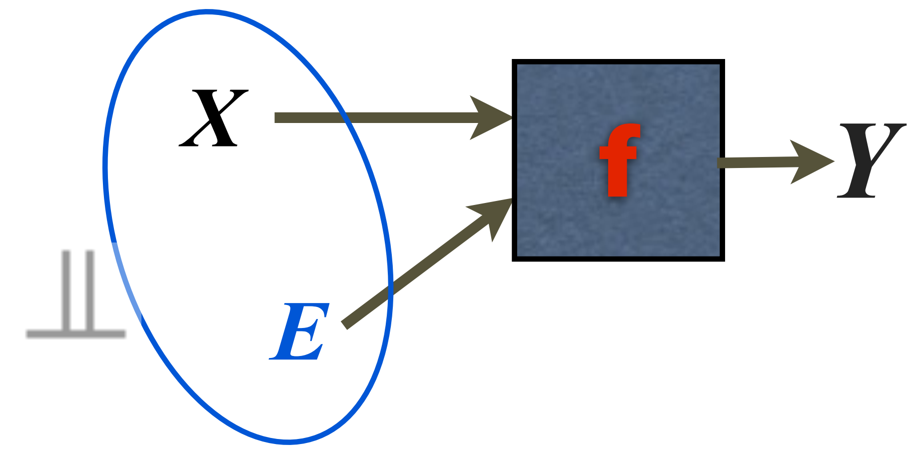


- :-(Without constraints on f, one can find independent noise for both directions (Darmois, 1951; Zhang et al., 2015)

  - Given any X_1 and X2, E' := conditional CDF of $X_2 \mid X_1$ is always independent from X_1 and $X2 = f(X_1, E')$

- :-) Structural constraints on f imply asymmetry

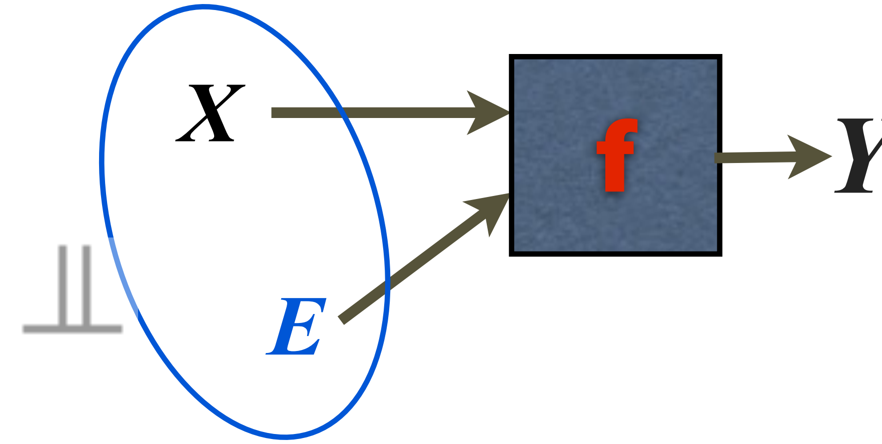
A Way to Construct Independent Error Term



- CDF(Y) is a random variable uniformly distributed over [0,1]
- $E' \triangleq$ Conditional CDF($Y \mid X=x$) is uniformly distributed over [0,1], irrelevant to the value of x
- $E' \perp\!\!\!\perp X$
- Y can be written as $Y = f(X, E')$, i.e., the transformation from (X, Y) to (X, E') is invertible
- Why? The Jacobin !

Zhang et al.(2015), On Estimation of Functional Causal Models: General Results and Application to Post-Nonlinear Causal Model, ACM Transactions on Intelligent Systems and Technology, Forthcoming

A Way to Construct Independent Error Term



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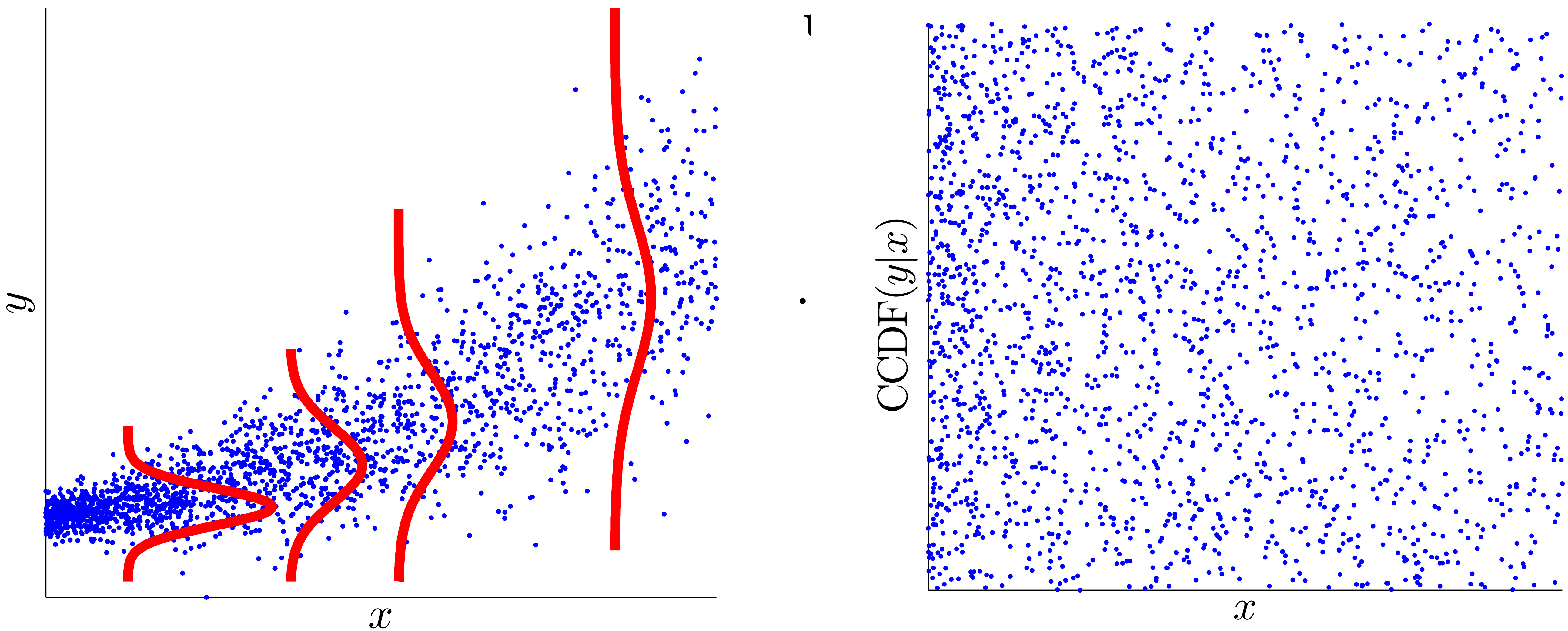

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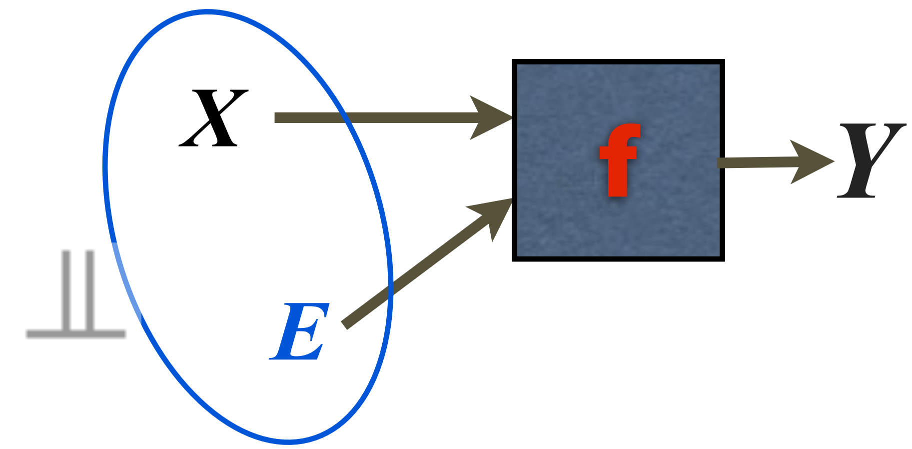

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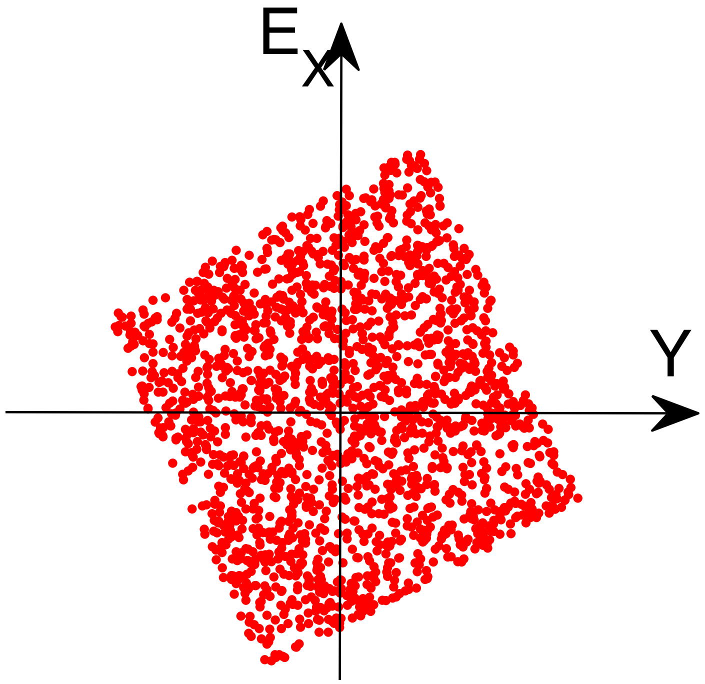
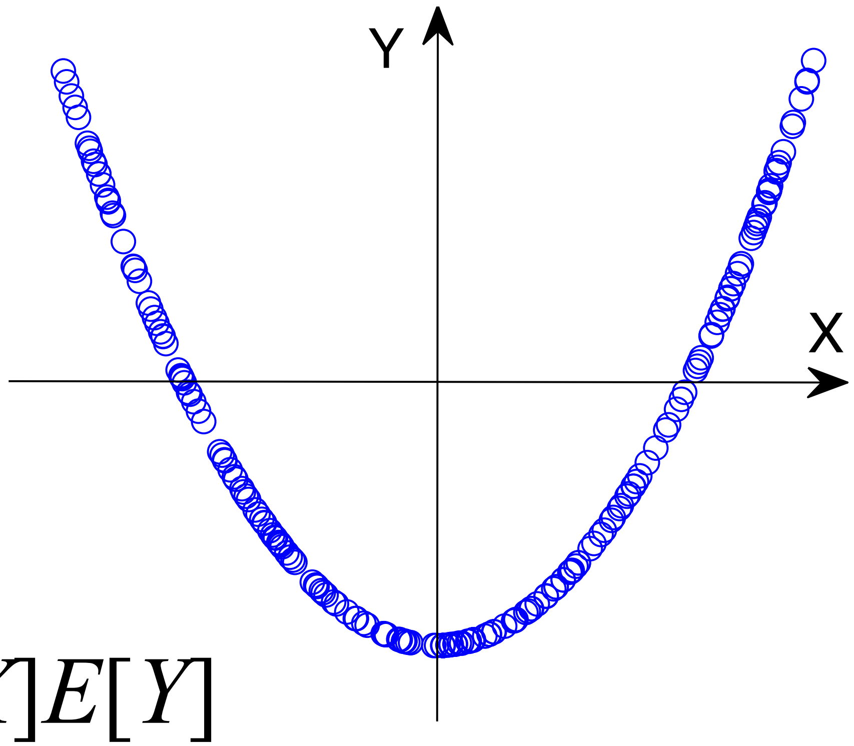
(Conditional) Independence

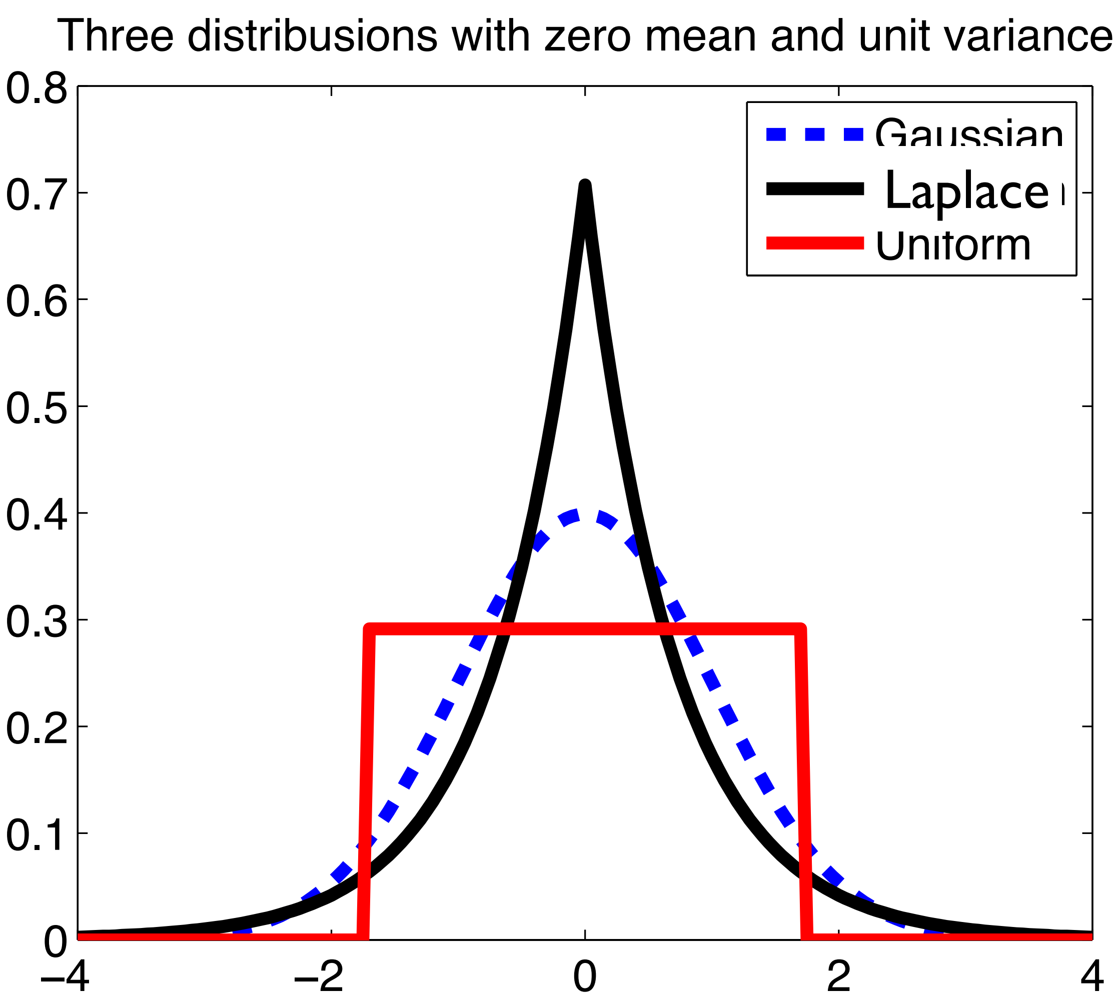
- $X \perp\!\!\!\perp Y$ iff $p(X,Y) = p(X)p(Y)$
  - or $p(X|Y) = P(X)$: Y not informative to X
- $\mathrm{X} \perp\!\!\!\perp \mathrm{Y} \mid \mathrm{Z}$ iff $p(X,Y|Z) = p(X|Z)p(Y|Z)$
  - or, $p(X|Y,Z) = p(X|Z)$: given Z, Y not informative to X
- Divide & conquer, remove irrelevant info…
- By construction, regression residual is uncorrelated (but not necessarily independent !) from the predictor

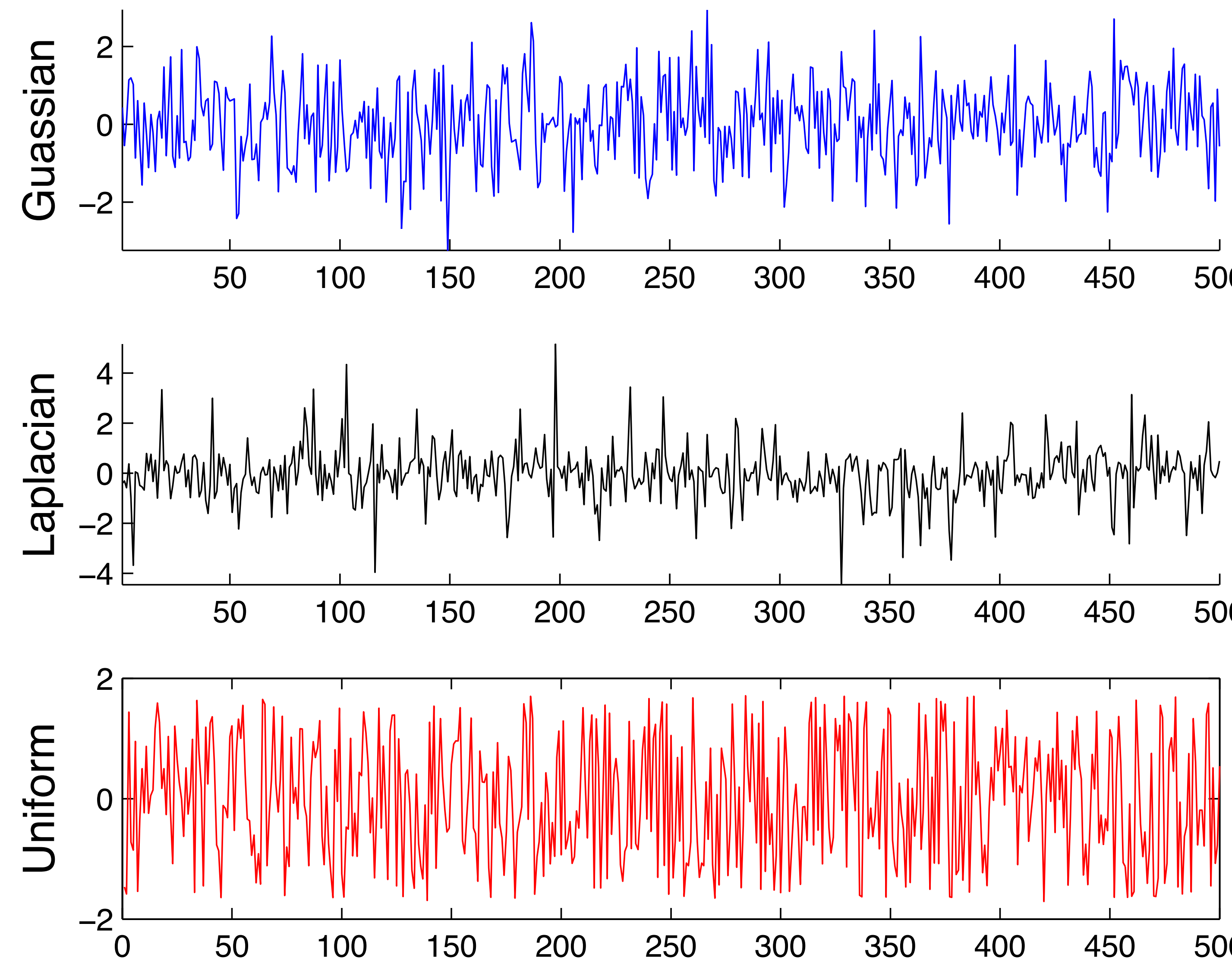




Uncorrelatedness: $E[XY] = E[X]E[Y]$

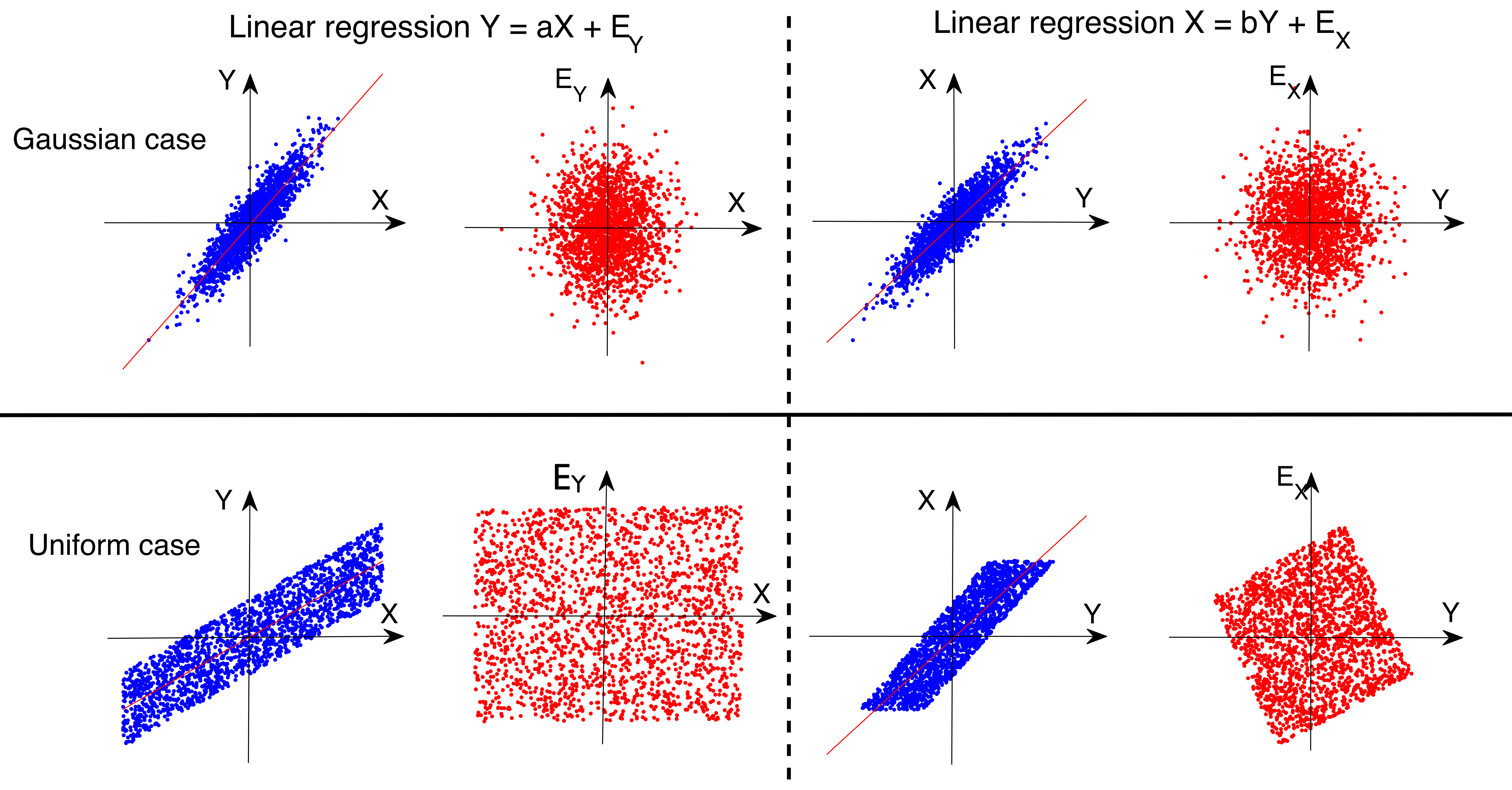
Gaussian vs. Non-Gaussian Distributions



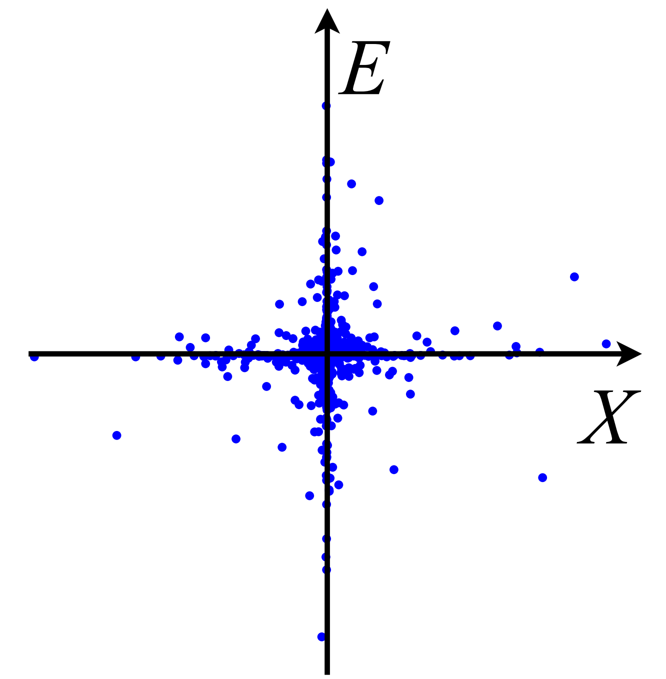


Causal Asymmetry the Linear Case: Illustration

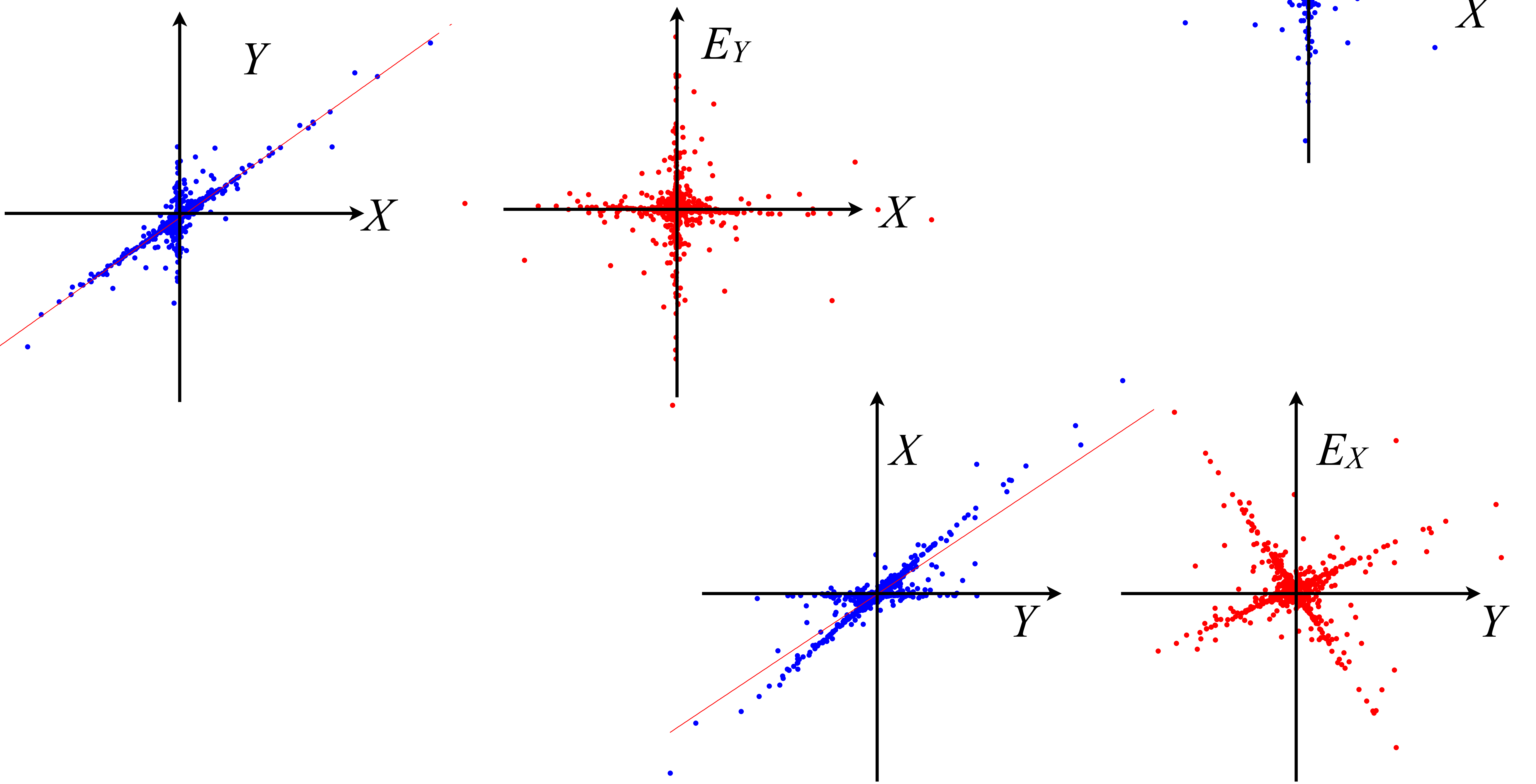
Data generated by $Y = aX + E$ (i.e., $X \to Y$):



Super-Gaussian Case



Data generated by $Y = aX + E$ ($X \rightarrow Y$):



More Generally, LiNGAM Model

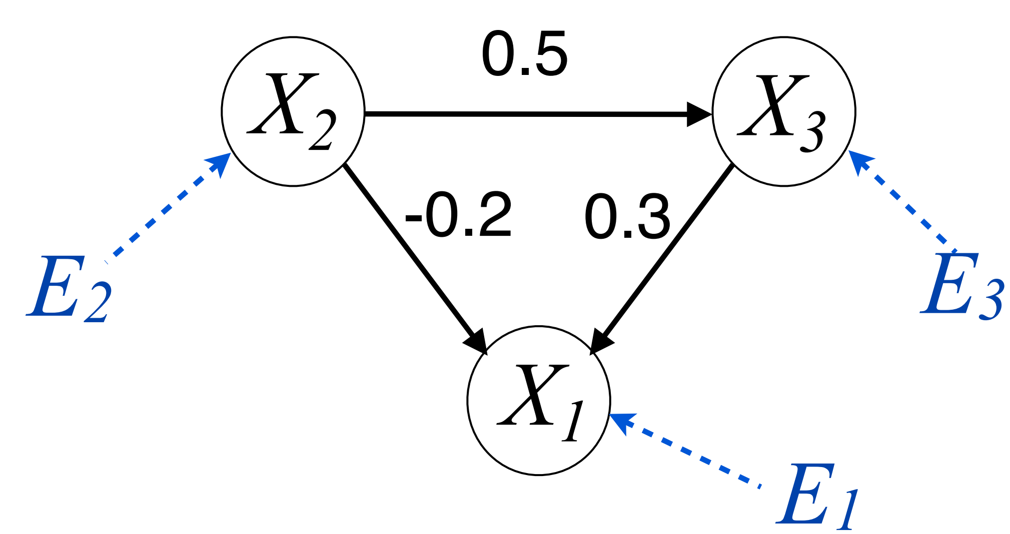
- Linear, non-Gaussian, acyclic causal model (LiNGAM) (Shimizu et al., 2006):

$$X_i = \sum_{j\text{: parents of } i} b_{ij} X_j + E_i \quad or \quad \mathbf{X} = \mathbf{B}\mathbf{X} + \mathbf{E}$$

  - Disturbances (errors) E_i are non-Gaussian (or at most one is Gaussian) and mutually independent

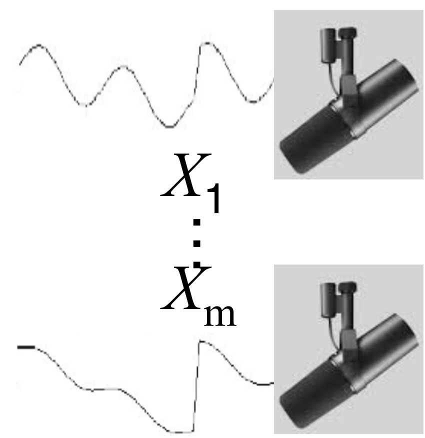
  - Example:

$$X_2 = E_2,$$
$$X_3 = 0.5X_2 + E_3,$$
$$X_1 = -0.2X_2 + 0.3X_3 + E_1.$$



Shimizu et al. (2006). A linear non-Gaussian acyclic model for causal discovery. Journal of Machine Learning Research, 7:2003–2030.

Independent Component Analysis



observed signals

$$\mathbf{X} = \mathbf{A} \cdot \mathbf{S} \qquad \mathbf{Y} = \mathbf{W} \cdot \mathbf{X}$$

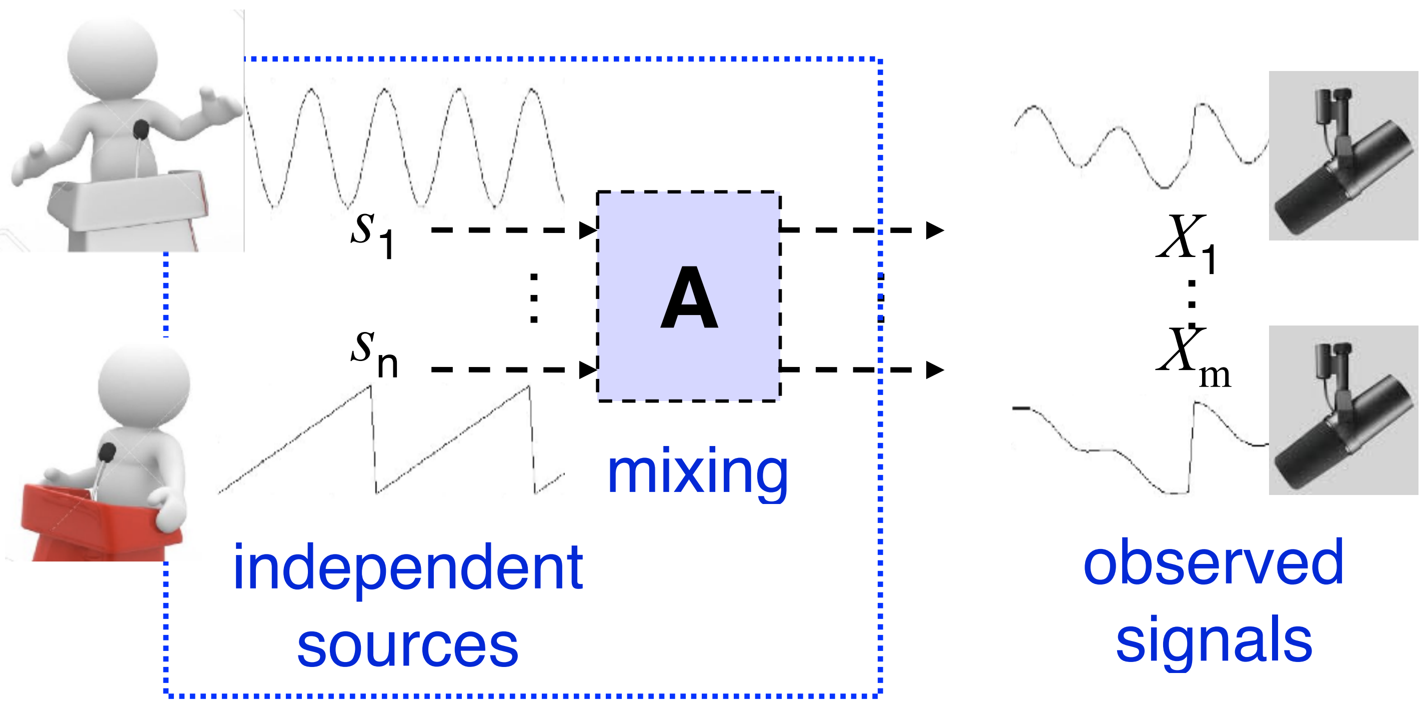
$$\begin{array}{c} X_1 \\ X_2 \end{array} \begin{bmatrix} .5 & .3 & 1.1 & -0.3 & \dots \\ .8 & -.7 & .3 & .5 & \dots \end{bmatrix} = \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}_{\mathbf{A}} \cdot \begin{bmatrix} ? & ? & ? & ? & \dots \\ ? & ? & ? & ? & \dots \end{bmatrix} \begin{array}{c} s_1 \\ s_2 \end{array}$$

- Assumptions in ICA
  - At most one of S_i is Gaussian
  - #Source <= # Sensor, and **A** is of full column rank

Then A can be estimated up to column scale and permutation indeterminacies

Hyvärinen et al., Independent Component Analysis, 2001

Independent Component Analysis



unknown mixing system

$$\mathbf{X} = \mathbf{A} \cdot \mathbf{S}$$

$$\mathbf{Y} = \mathbf{W} \cdot \mathbf{X}$$

$$\begin{array}{c} X_1 \\ X_2 \end{array} \begin{bmatrix} .5 & .3 & 1.1 & -0.3 & \dots \\ .8 & -.7 & .3 & .5 & \dots \end{bmatrix} = \underbrace{\begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}}_{A} \cdot \begin{bmatrix} ? & ? & ? & ? & \dots \\ ? & ? & ? & ? & \dots \end{bmatrix} \begin{array}{c} s_1 \\ s_2 \end{array}$$

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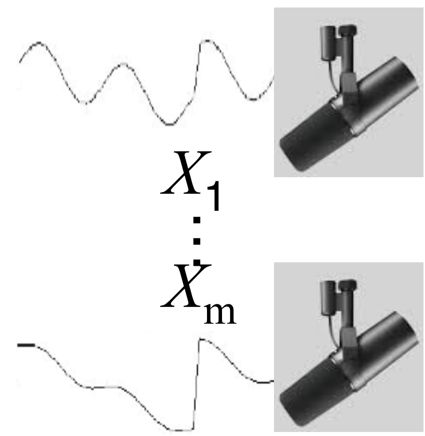
Hyvärinen et al., Independent Component Analysis, 2001

Independent Component Analysis



observed signals

$$\mathbf{X} = \mathbf{A} \cdot \mathbf{S} \qquad\qquad \mathbf{Y} = \mathbf{W} \cdot \mathbf{X}$$

$$\begin{array}{c} X_1 \\ X_2 \end{array} \begin{bmatrix} .5 & .3 & 1.1 & -0.3 & \dots \\ .8 & -.7 & .3 & .5 & \dots \end{bmatrix} = \underbrace{\begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}}_{A} \cdot \begin{bmatrix} ? & ? & ? & ? & \dots \\ ? & ? & ? & ? & \dots \end{bmatrix} \begin{array}{c} s_1 \\ s_2 \end{array}$$

- Assumptions in ICA
  - At most one of S_i is Gaussian
  - #Source <= # Sensor, and **A** is of full column rank

Then A can be estimated up to column scale and permutation indeterminacies

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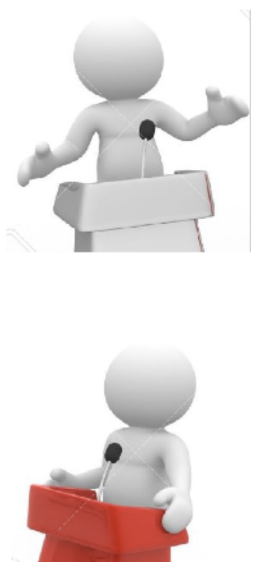

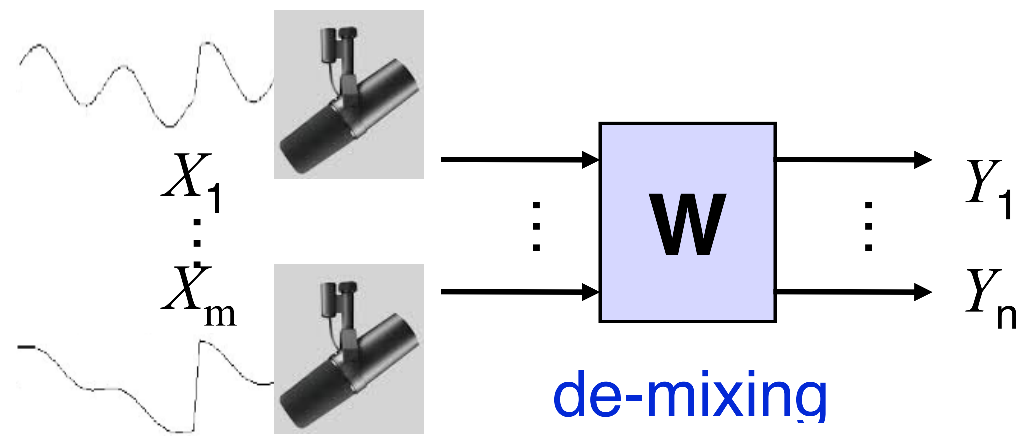

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ICA system

output: as independent as possible

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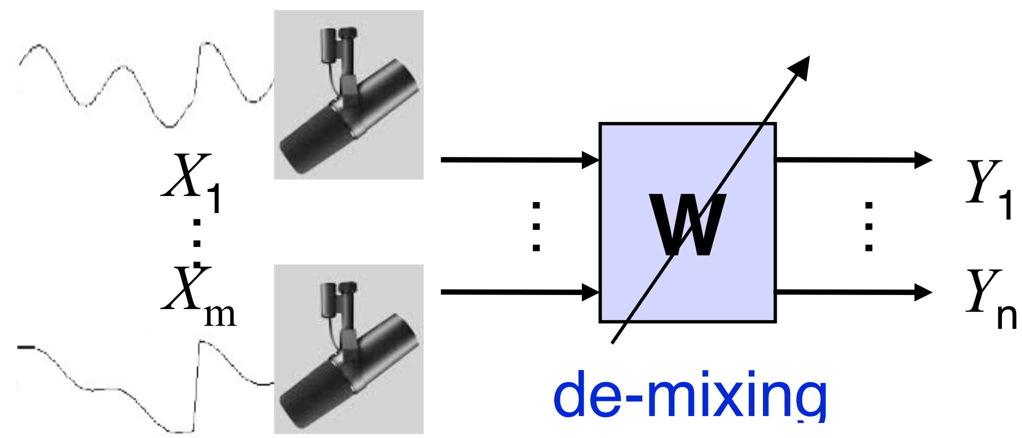

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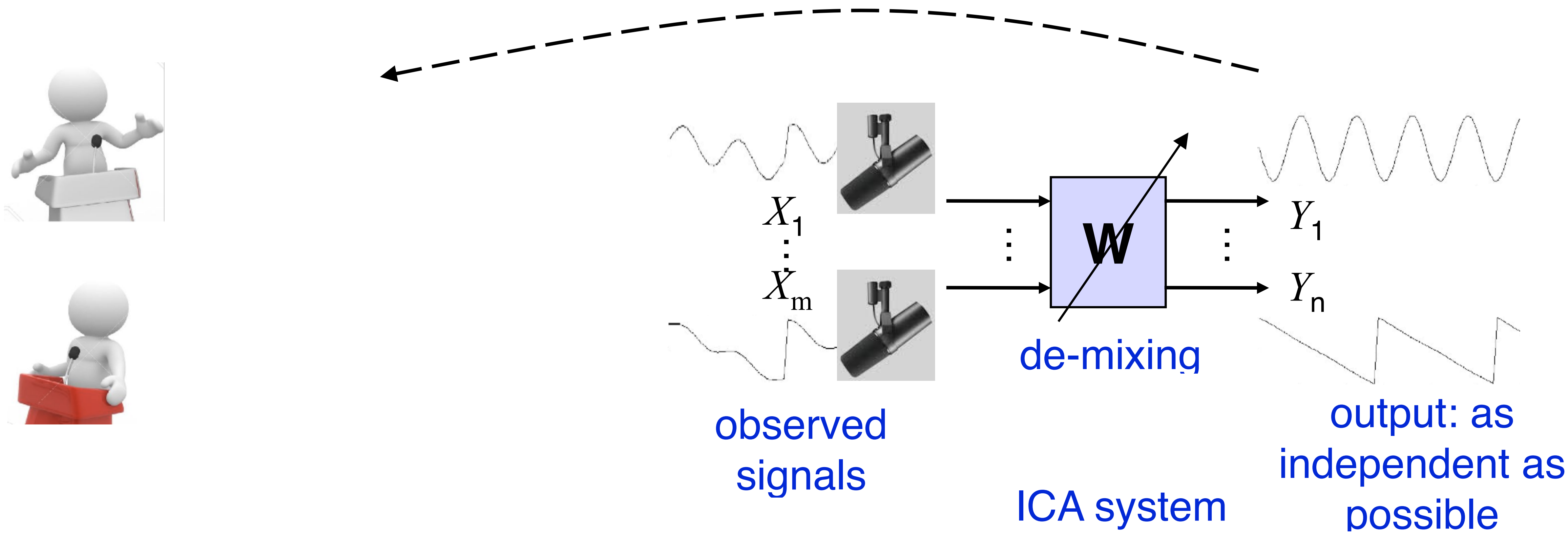

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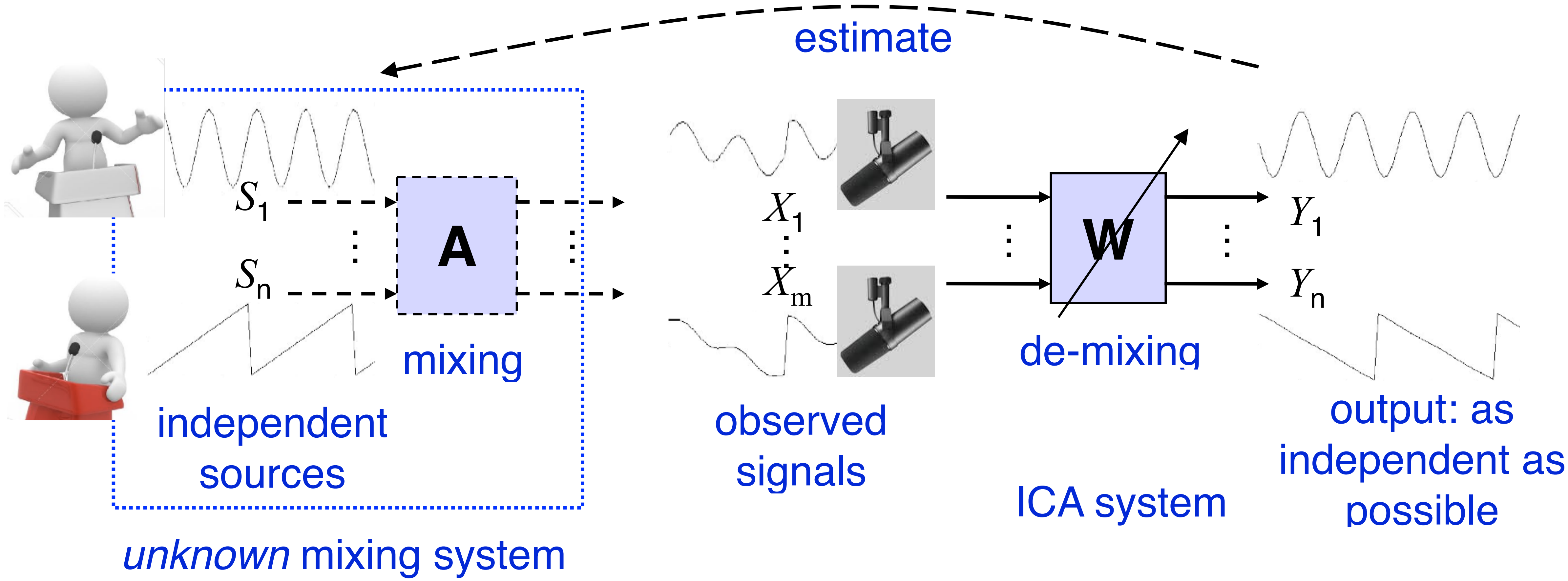

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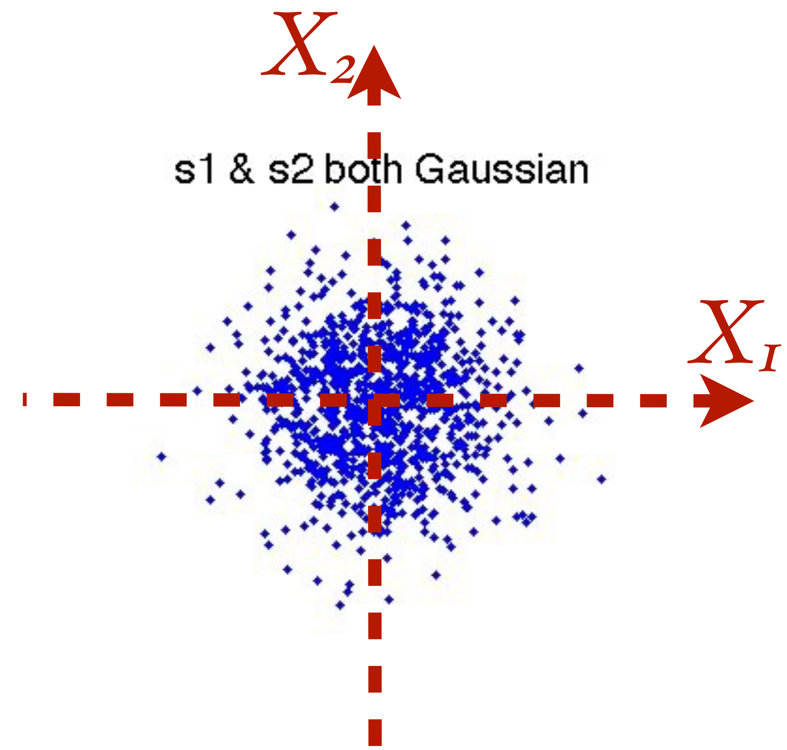
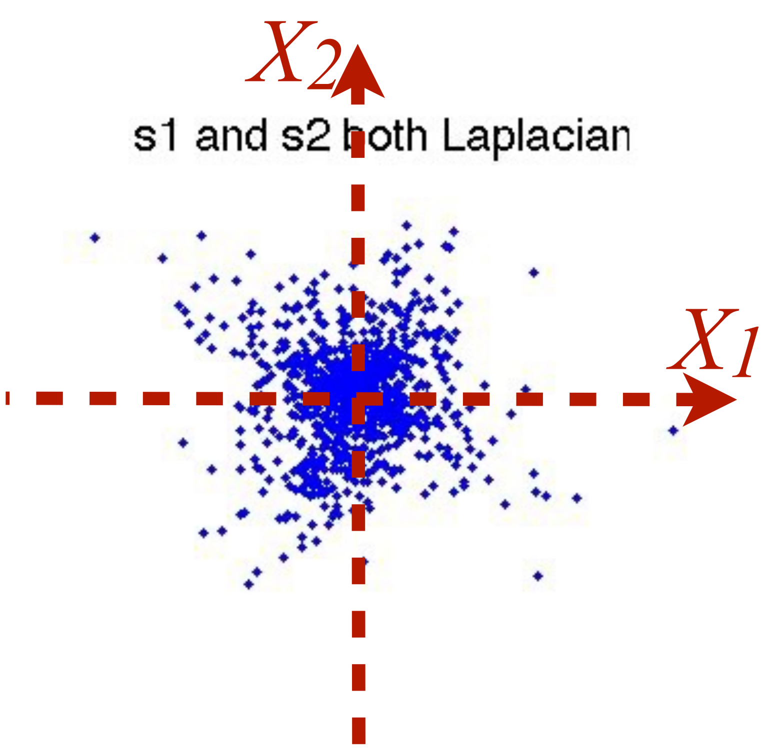
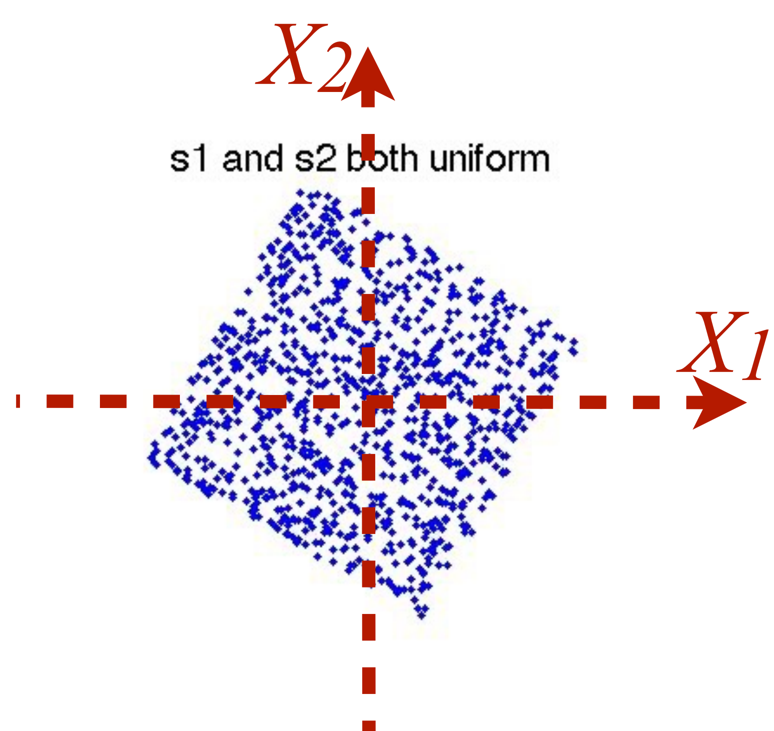
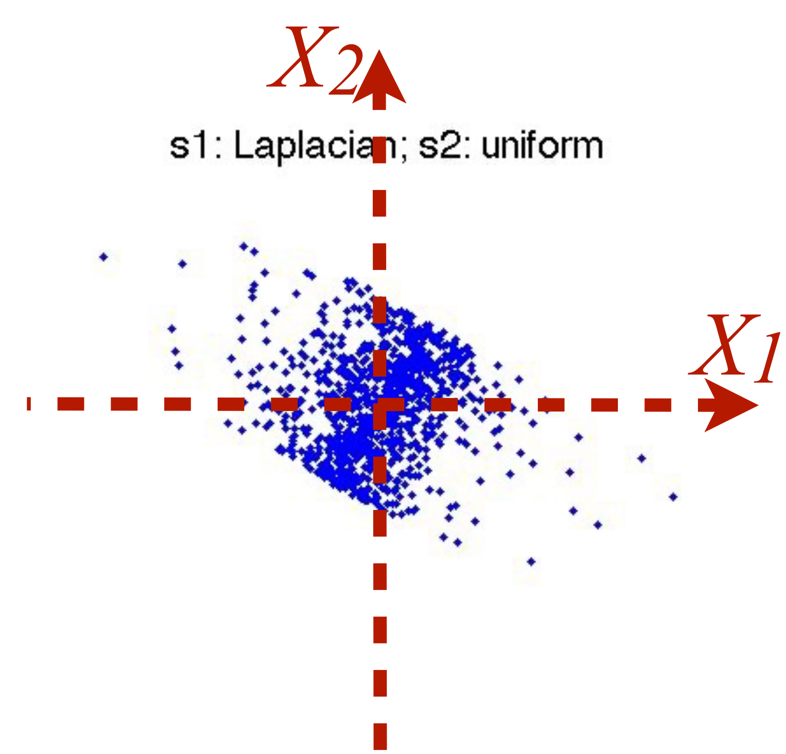
Intuition: Why ICA works?

- (After preprocessing) ICA aims to find a rotation transformation $\mathbf{Y} = \mathbf{W} \cdot \mathbf{X}$ to making Y_i independent
  - By maximum likelihood $\log p(X|\boldsymbol{A})$, mutual information $MI(Y_1,\ldots,Y_m)$ minimization, infomax...









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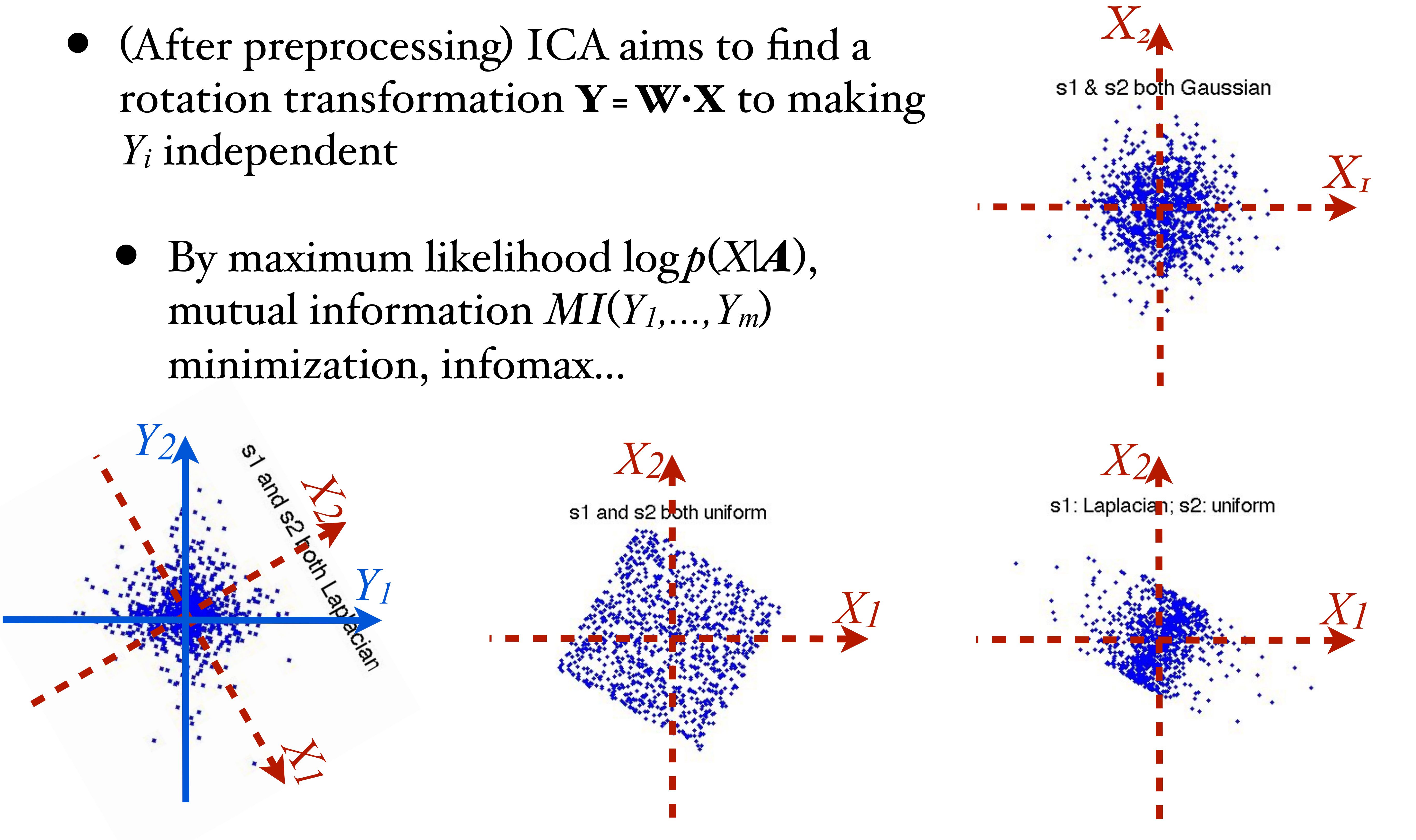

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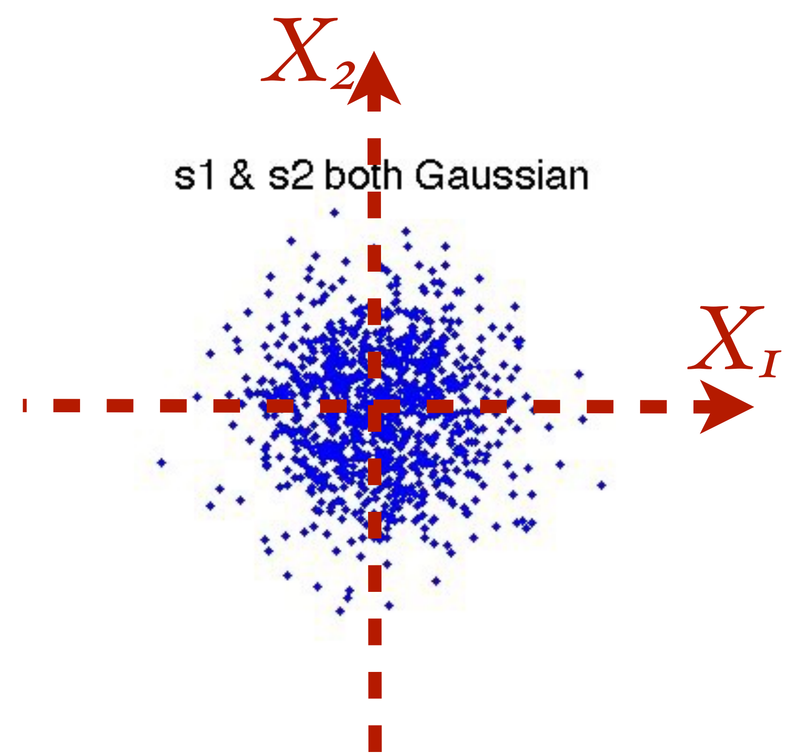

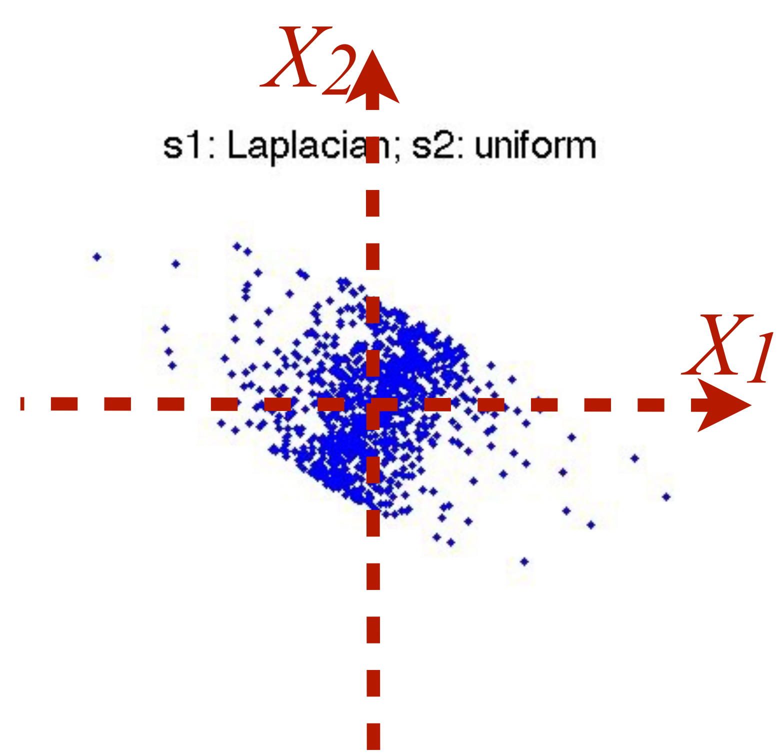

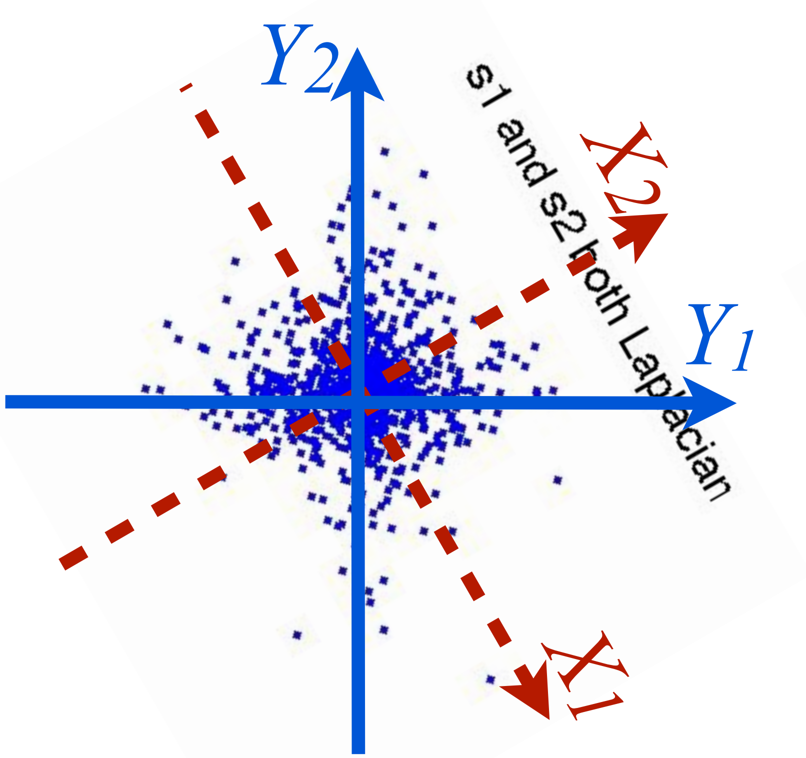

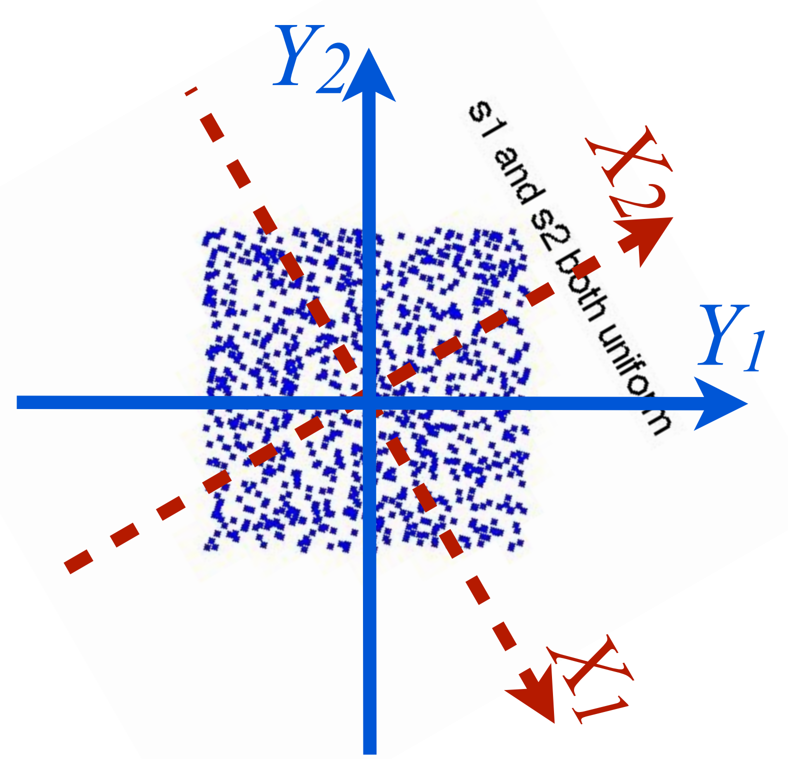

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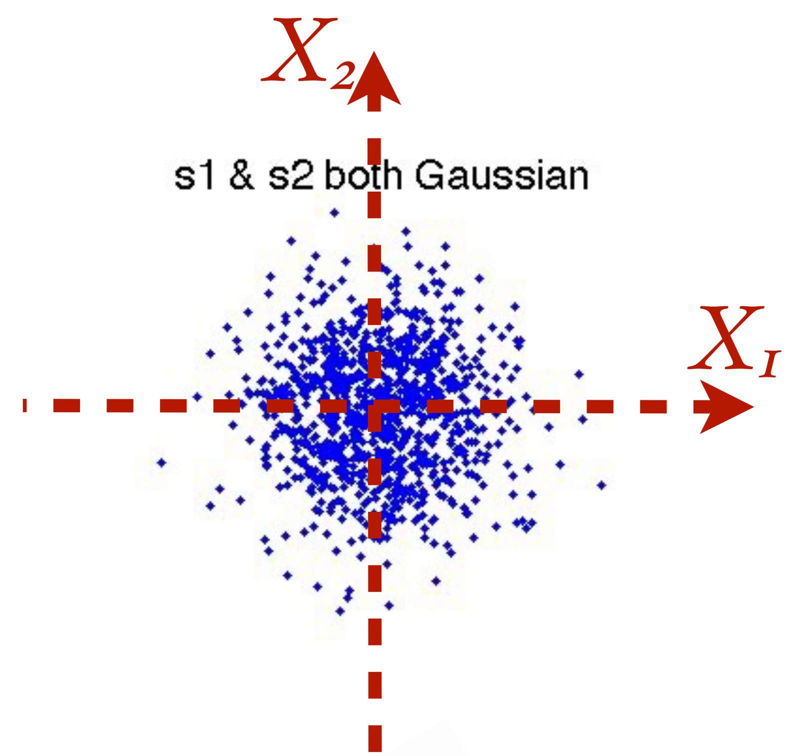
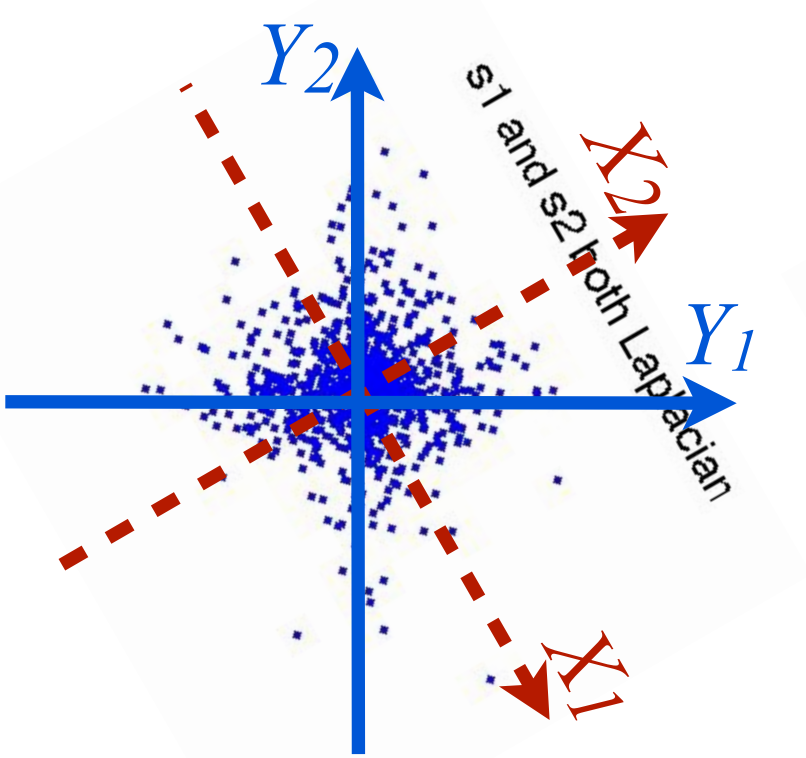
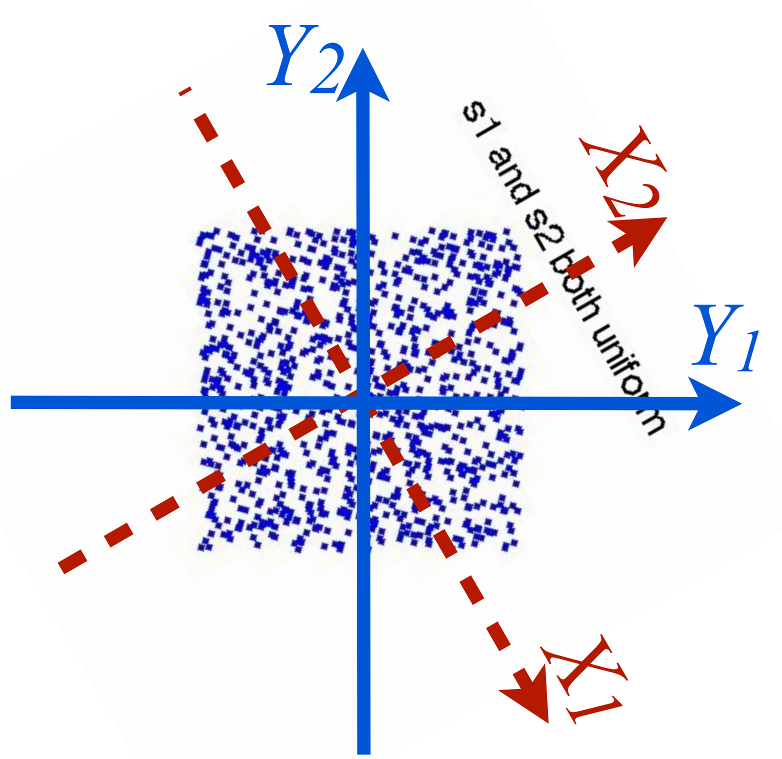
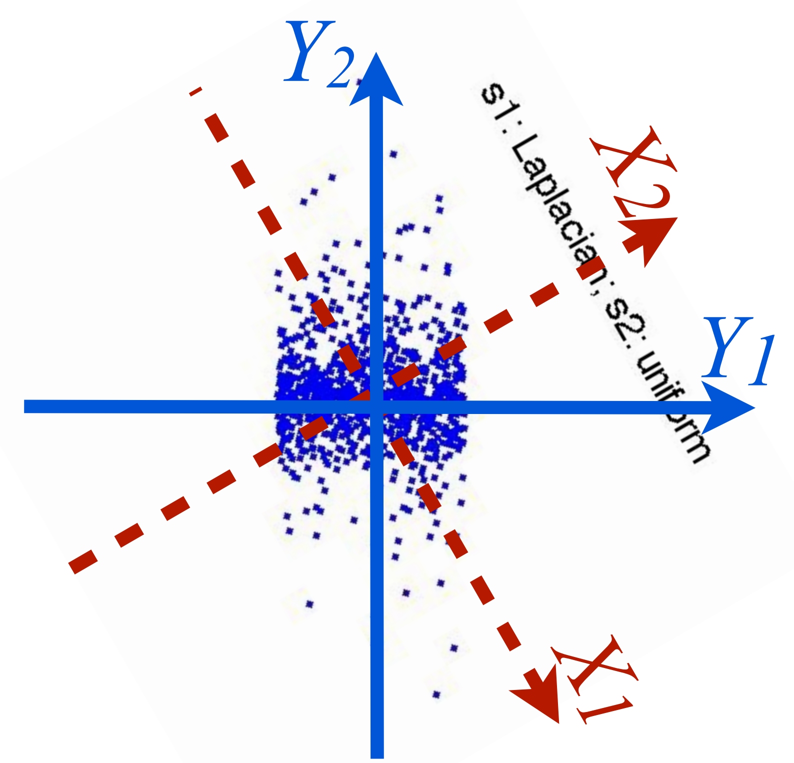
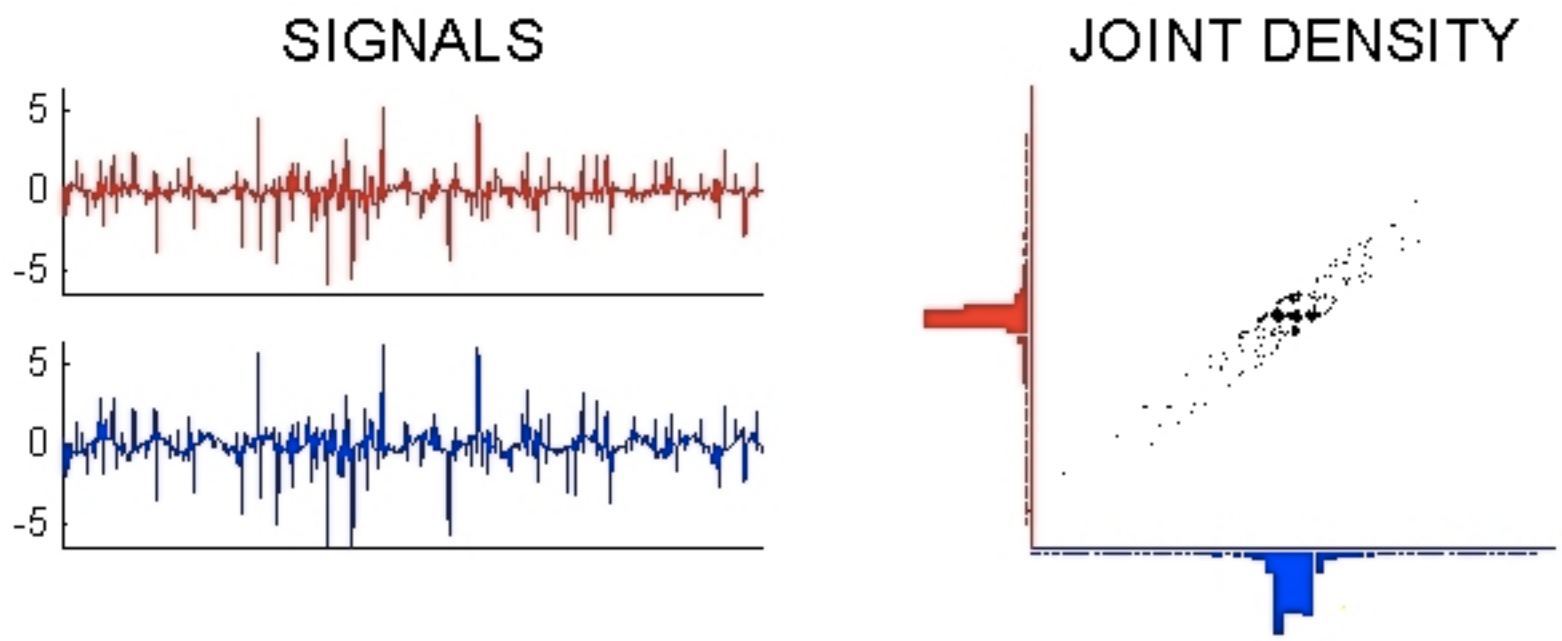




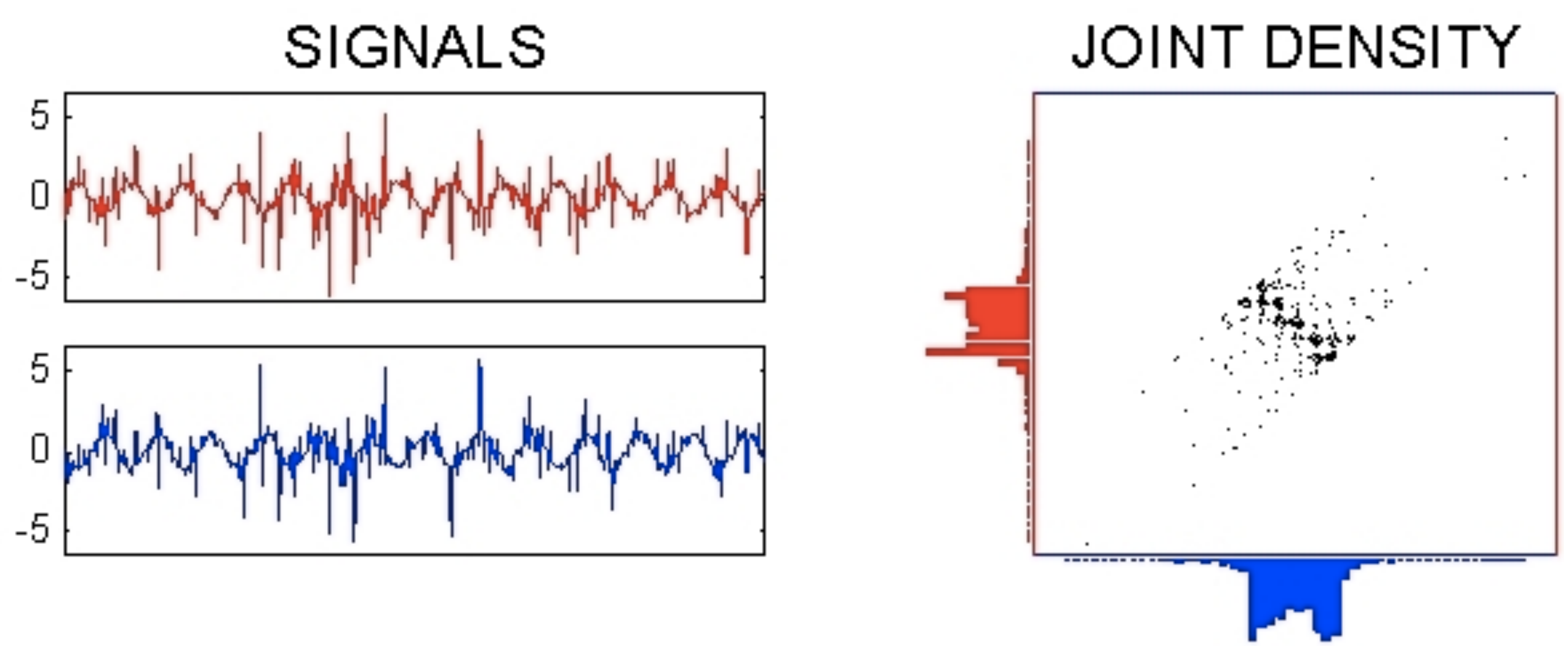




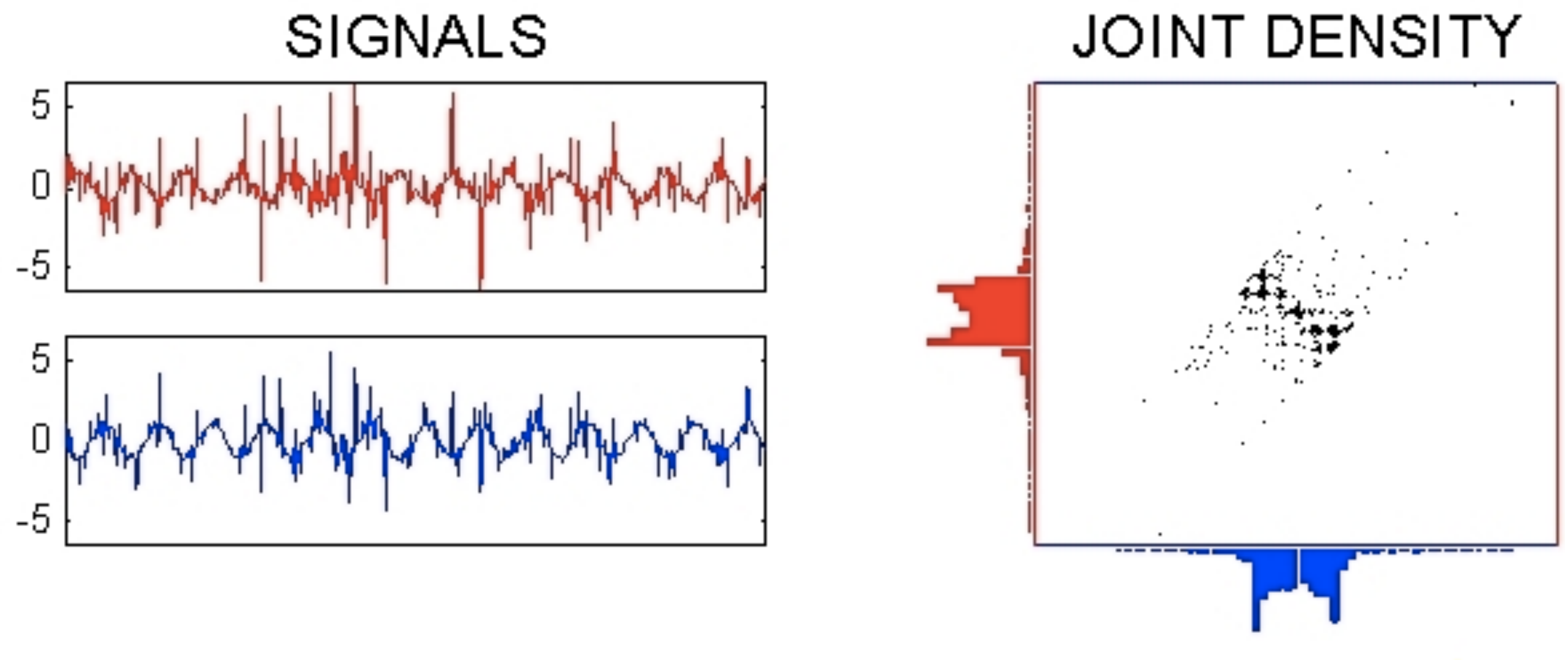
A Demo of the ICA Procedure



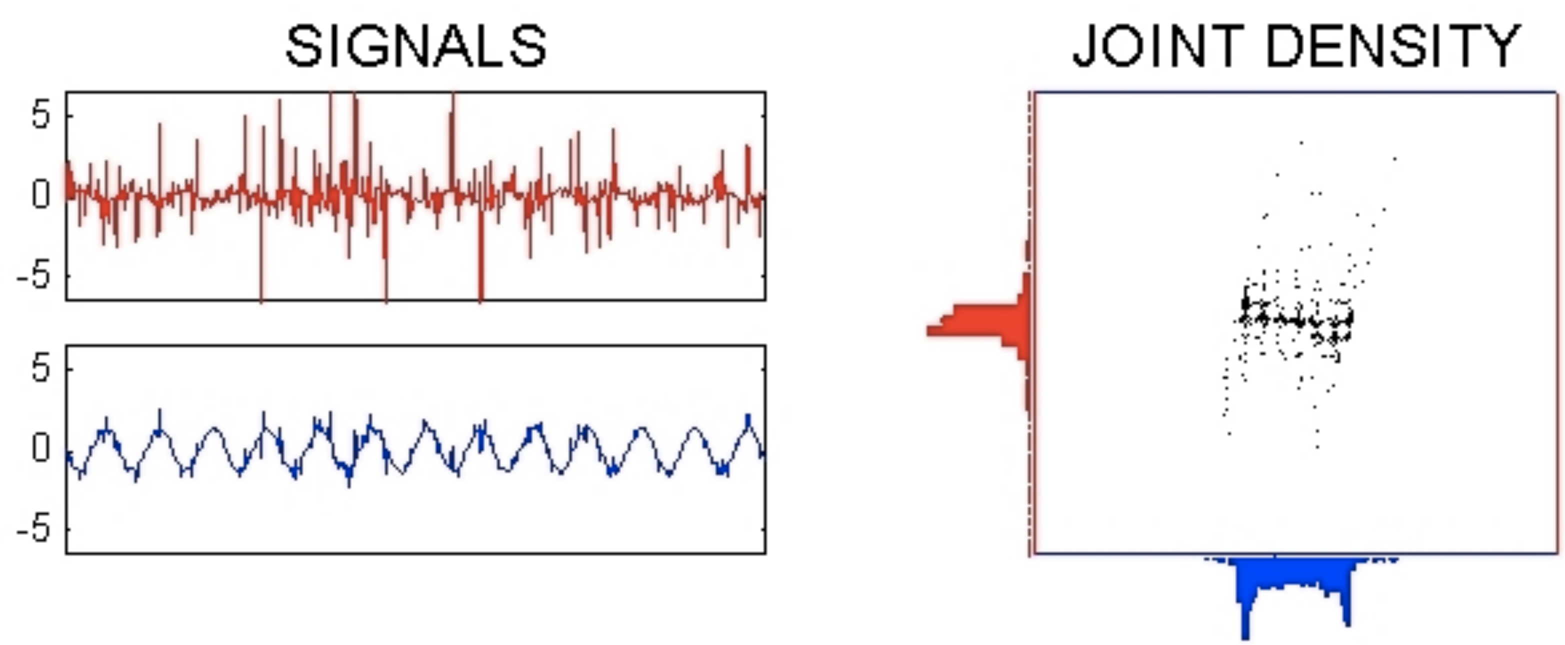
Input signals and density



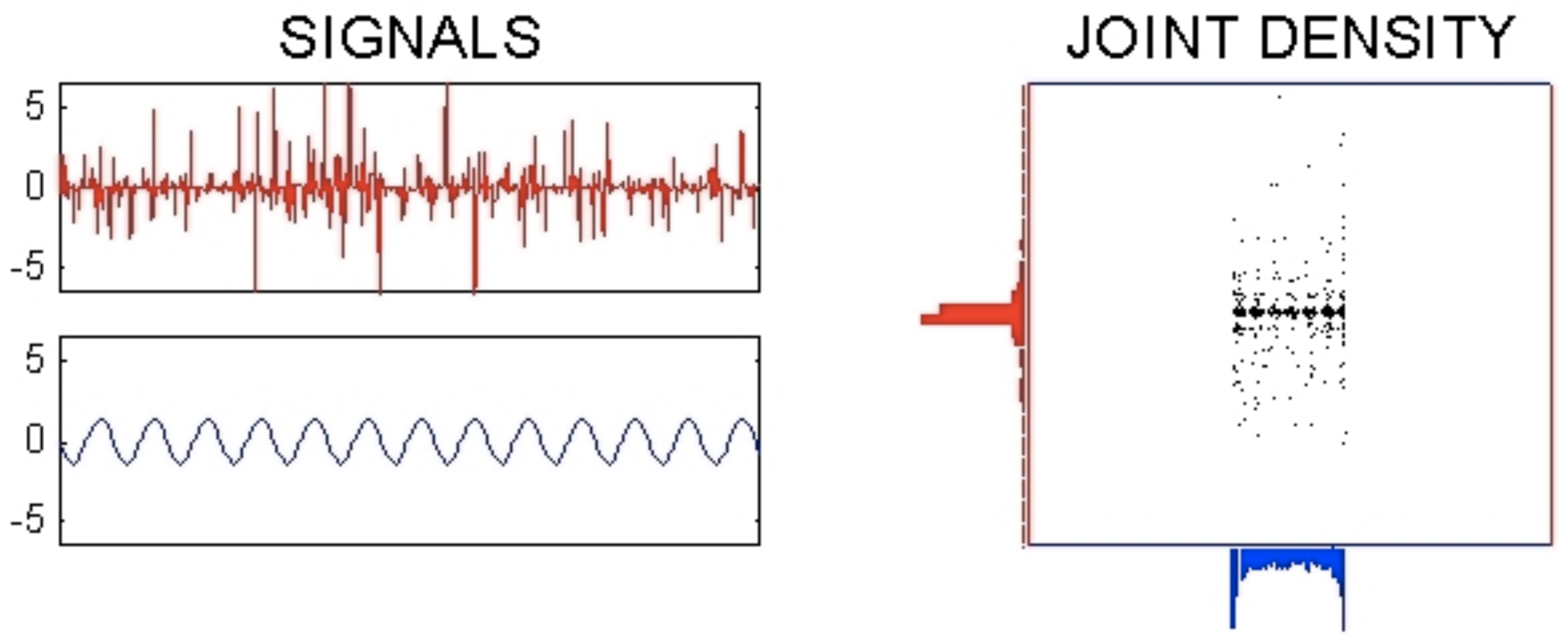
Whitened signals and density



Separated signals after 1 step of FastICA



Separated signals after 3 steps of FastICA



Separated signals after 5 steps of FastICA

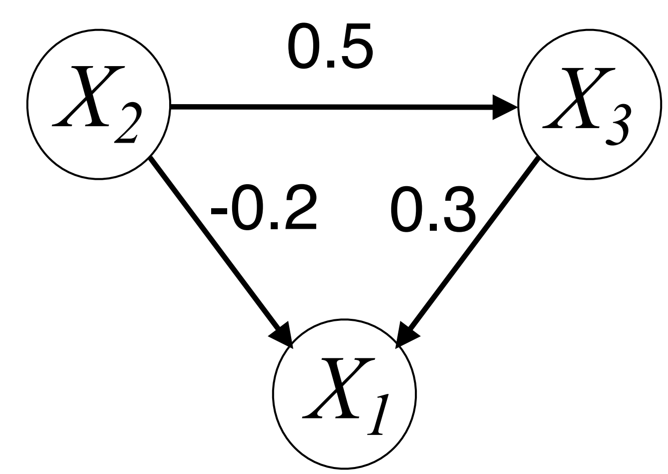
LiNGAM Analysis by ICA

- LiNGAM: $X_i = \sum_{j:\ \text{parents of } i} b_{ij} X_j + E_i \quad \textit{or} \quad \mathbf{X} = \mathbf{B}\mathbf{X} + \mathbf{E} \Rightarrow \mathbf{E} = (\mathbf{I}-\mathbf{B})\mathbf{X}$
  - $\mathbf{B}$ has special structure: acyclic relations
- ICA: $\mathbf{Y} = \mathbf{W}\mathbf{X}$
- $\mathbf{B}$ can be seen from $\mathbf{W}$ by permutation and re-scaling
- Faithfulness assumption avoided
- E.g.,

$$\begin{bmatrix} E_1 \\ E_3 \\ E_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ -0.5 & 1 & 0 \\ 0.2 & -0.3 & 1 \end{bmatrix} \cdot \begin{bmatrix} X_2 \\ X_3 \\ X_1 \end{bmatrix}$$

$$\Leftrightarrow \begin{cases} X_2 = E_1 \\ X_3 = 0.5X_2 + E_3 \\ X_1 = -0.2X_2 + 0.3X_3 + E_2 \end{cases}$$

So we have the causal relation:



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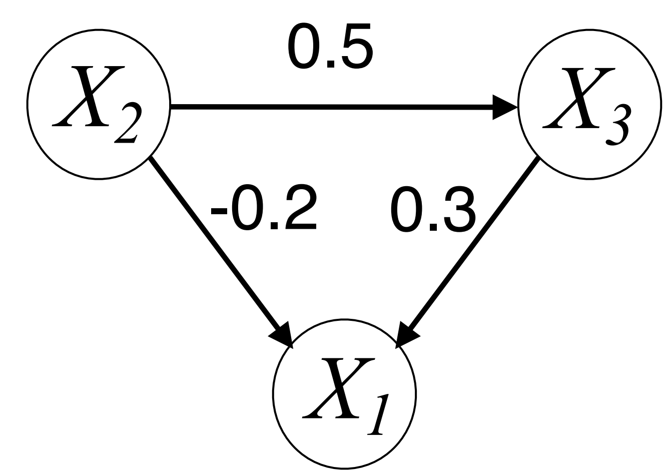

Question 1. How to find W?

Question 2. How to see B from W?

LiNGAM Analysis by ICA

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1. First permute the rows of **W** to make all diagonal entries non-zero, yielding $\ddot{\mathbf{W}}$.
2. Then divide each row of $\ddot{\mathbf{W}}$ by its diagonal entry, giving $\ddot{\mathbf{W}}$'.
3. $\hat{\mathbf{B}} = \mathbf{I} - \ddot{\mathbf{W}}'$.

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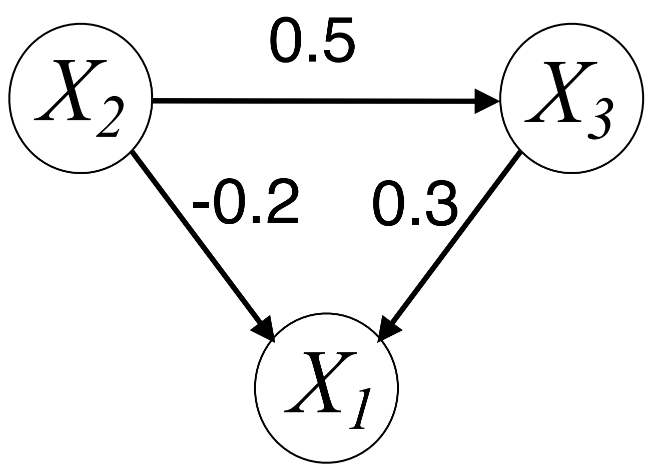

Can You See Causal Relations from $\mathbf{W}$? Example

- ICA gives $\mathbf{Y} = \mathbf{W}\mathbf{X}$ and

$$\mathbf{W} = \begin{bmatrix} 0.6 & -0.4 & 2 & 0 \\ 1.5 & 0 & 0 & 0 \\ 0 & 0.2 & 0 & 0.5 \\ 1.5 & 3 & 0 & 0 \end{bmatrix}$$

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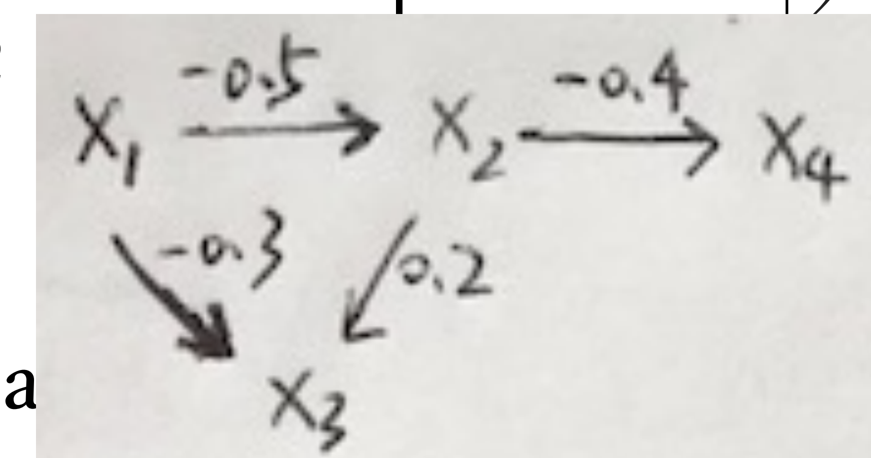

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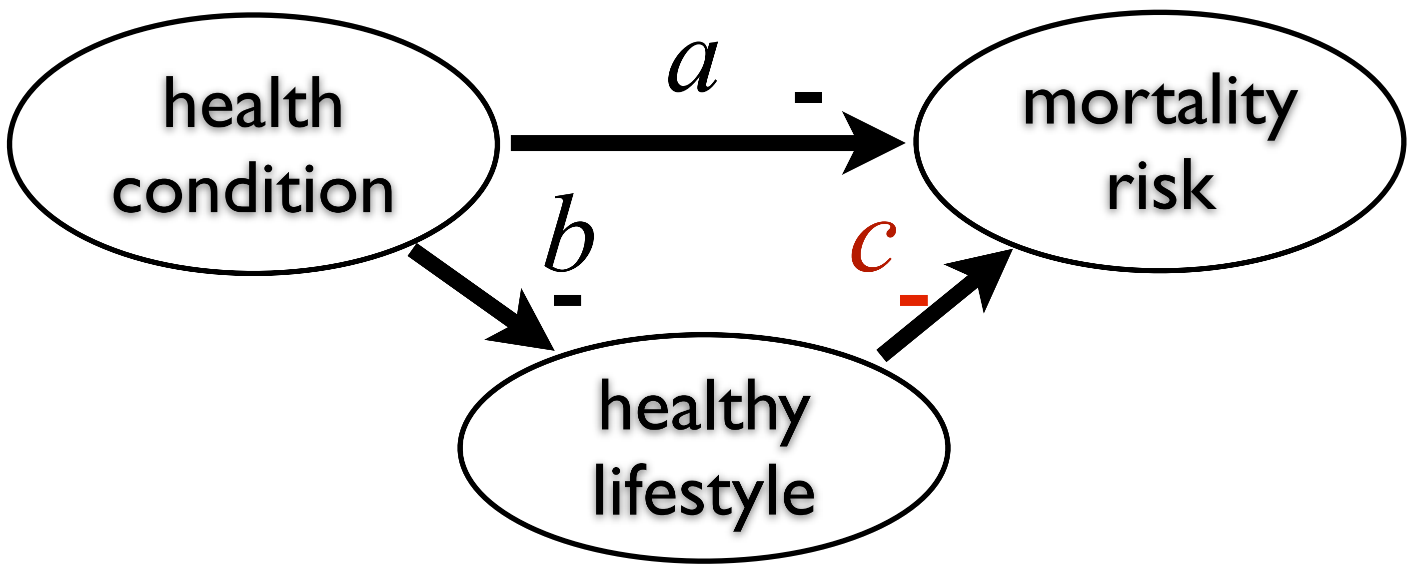
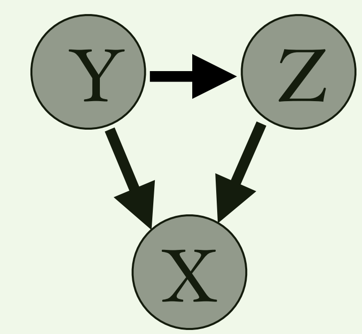
Faithfulness Assumption Needed?

- One might find independence between health condition & risk of mortality. Why?





Possible to have $Y \perp\!\!\!\perp Z \mid X$?

- E.g., if $a=-bc$, then *health_condition* $\perp\!\!\!\perp$ *mortality_risk*, which cannot by seen from the graph!
- No faithfulness assumption is needed in LiNGAM
  - Minimality (a zero coefficient corresponds to edge absence) is sufficient

Step-by-Step Demo & Application

- Galton family height data
- Result of PC?
- Linear, non-Gaussian methods: let's do causal discovery step by step with 'illust_LiNGAM_Galton.m'

Galton's height data

family	father	mother	Gender	Height
1	78.5	67	0	73.2
1	78.5	67	1	69.2
1	78.5	67	1	69
1	78.5	67	1	69
2	75.5	66.5	0	73.5
2	75.5	66.5	0	72.5
2	75.5	66.5	1	65.5
2	75.5	66.5	1	65.5
3	75	64	0	71
3	75	64	1	68
4	75	64	0	70.5
4	75	64	0	68.5
4	75	64	1	67
4	75	64	1	64.5
...	...	...	...	...

*

Some Estimation Methods for LiNGAM

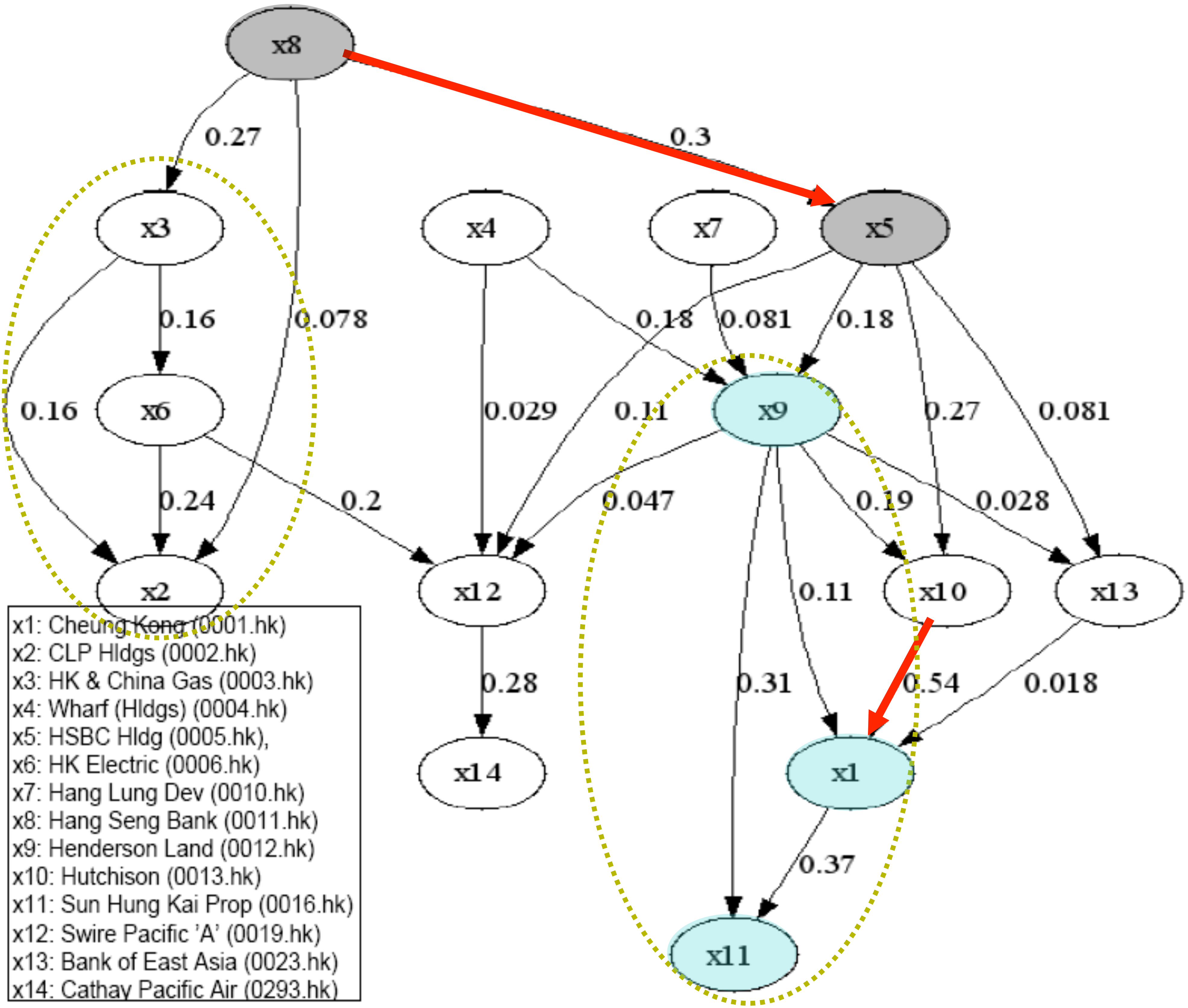
- ICA-LiNGAM
- ICA with Sparse Connections
- DirectLiNGAM...

Shimizu et al. (2006). A linear non-Gaussian acyclic model for causal discovery. Journal of Machine Learning Research, 7:2003–2030.

Zhang et al. (2006) ICA with sparse connections: Revisited. Lecture Notes in Computer Science, 5441:195–202, 2009

Shimizu, et al. (2011). DirectLiNGAM: A direct method for learning a linear non-Gaussian structural equation model. Journal of Machine Learning Research, 12:1225–1248.

Application: Causal diagram in HK Stock Market (Zhang & Chan, 2006)



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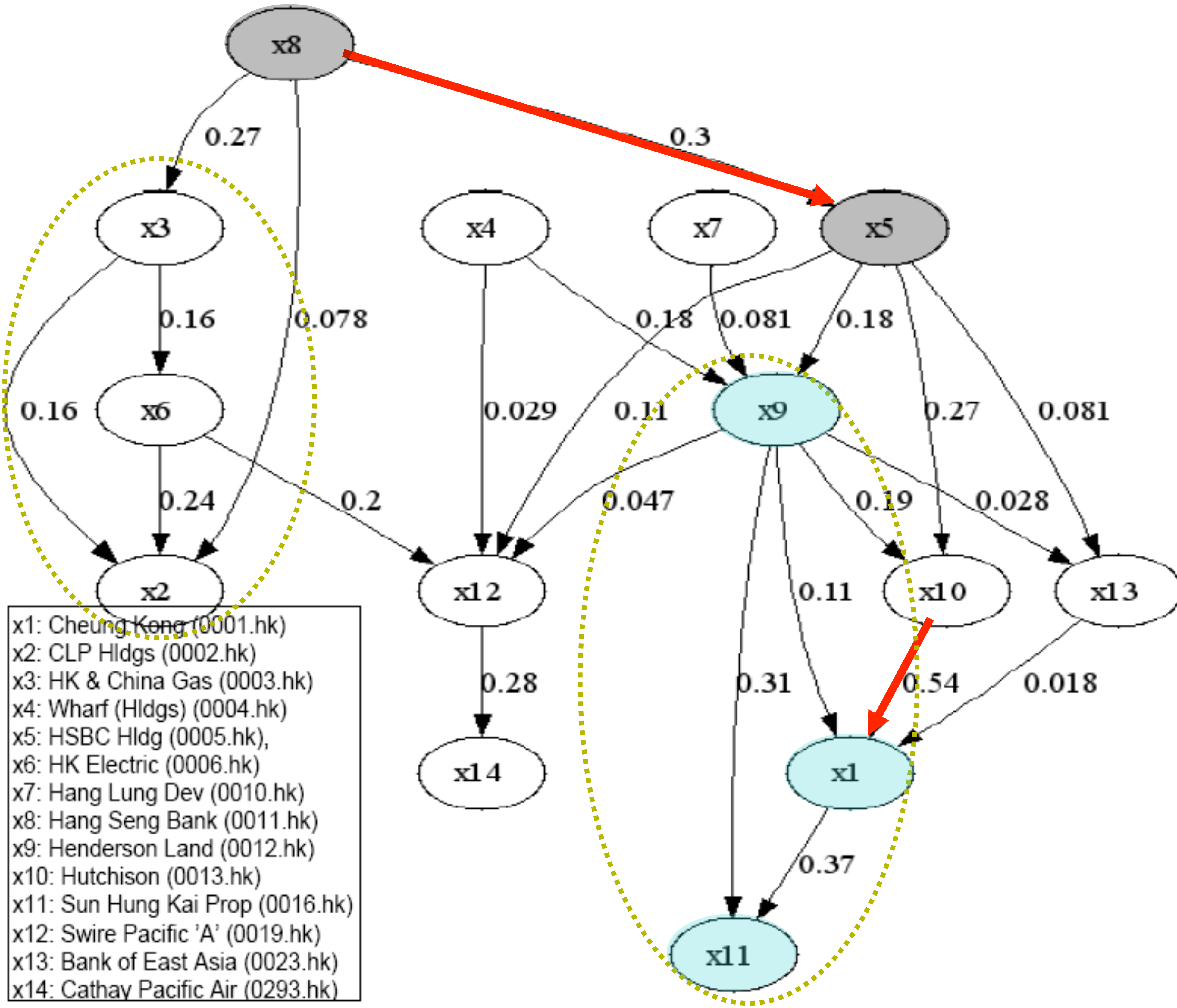

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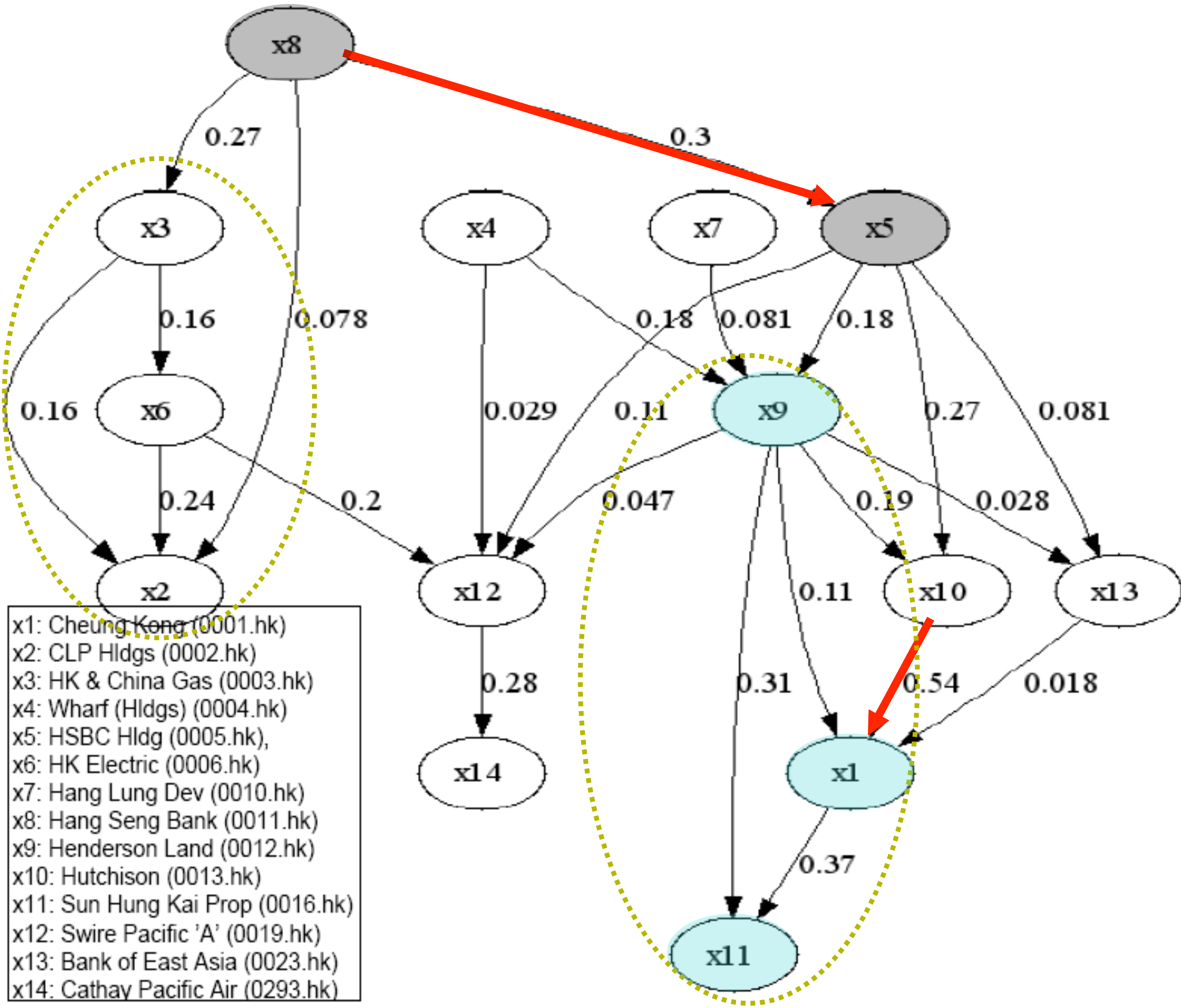

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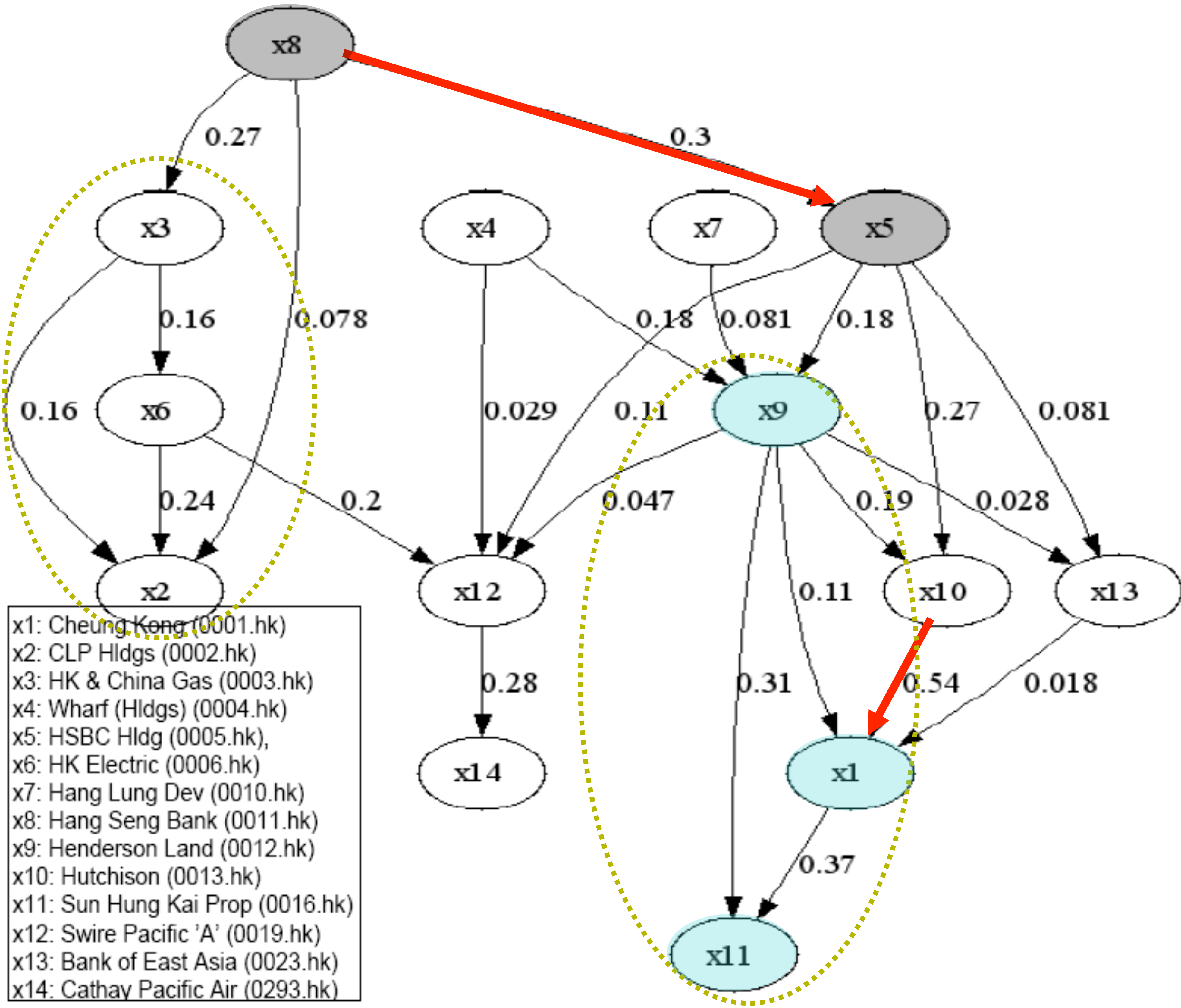

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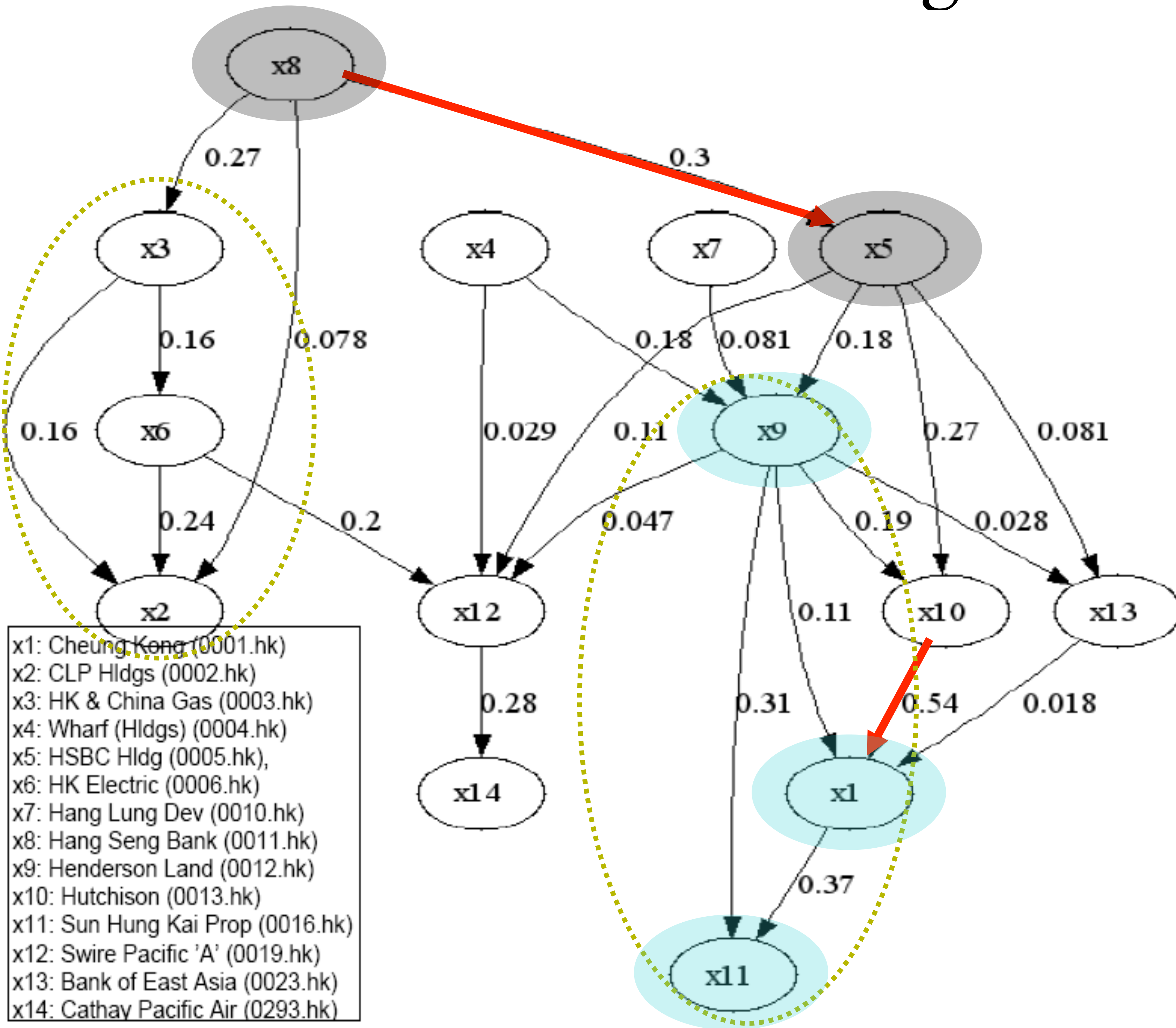

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4. Stocks in Property Index (x1, x9, x11) depend on many stocks, while they hardly influence others.

Independent Noise (IN) Condition

$$\mathbf{Z} \longrightarrow Y$$

- $(\mathbf{Z}, Y)$ follows the <u>IN condition</u> iff regression residual $Y - \tilde{w}^\intercal \mathbf{Z}$ is independent from $\mathbf{Z}$
- Estimate the Linear, Non-Gaussian Acyclic Causal model (LiNGAM), because $(\mathbf{Z}, Y)$ satisfies the IN condition iff
  - All variables in $\mathbf{Z}$ are causally earlier than Y &
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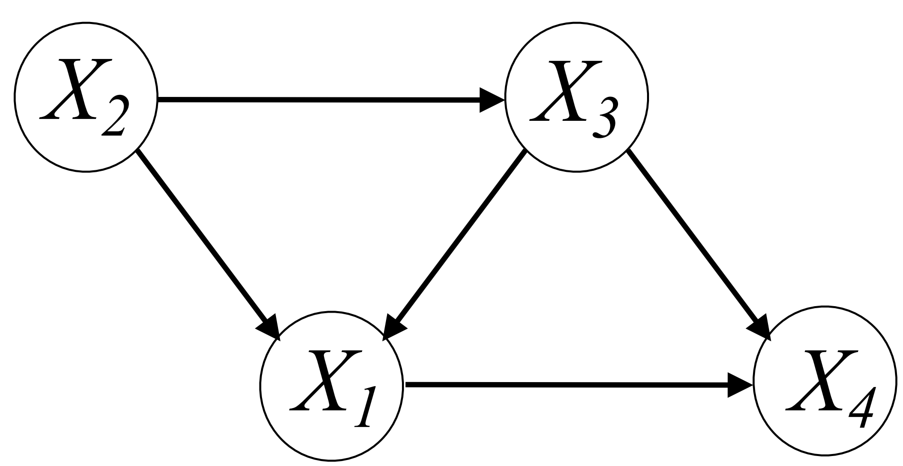

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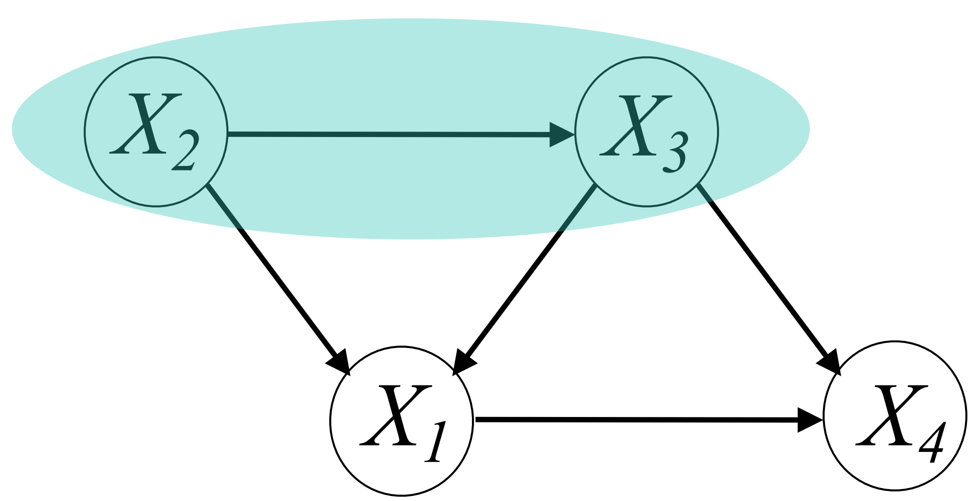

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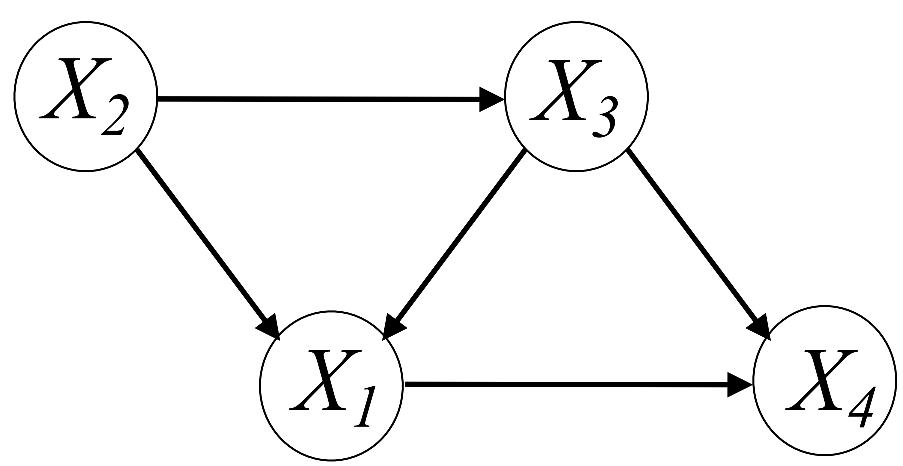

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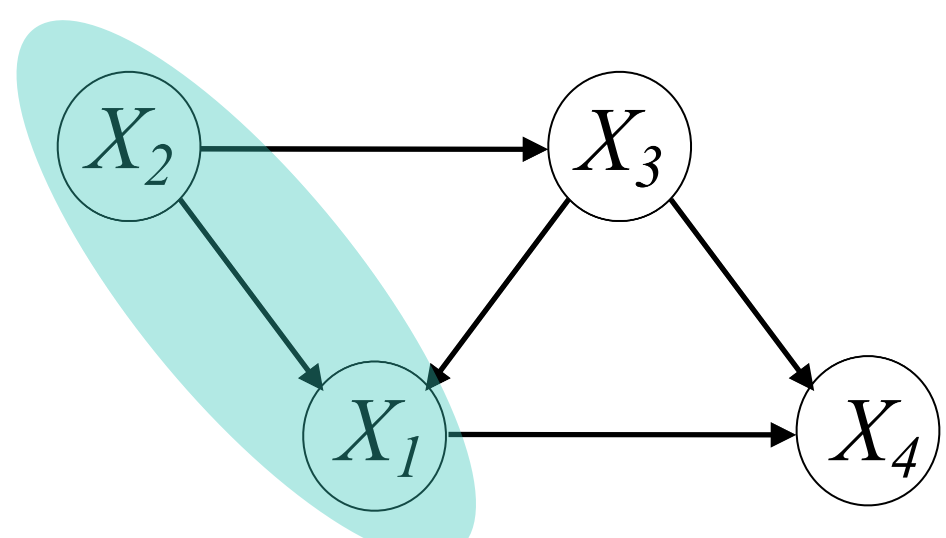

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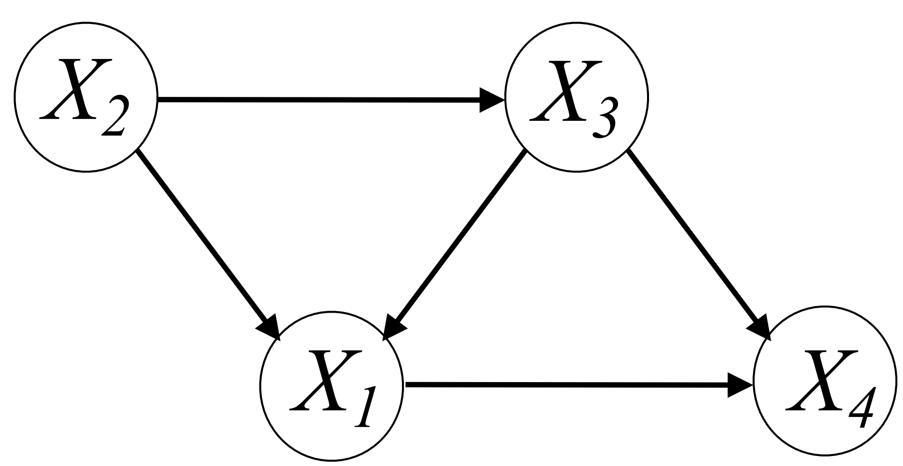

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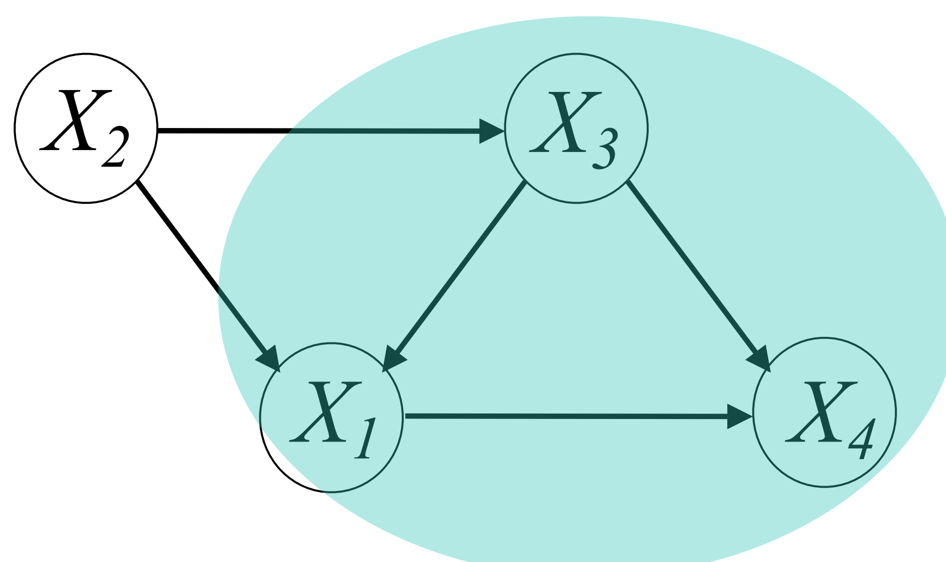

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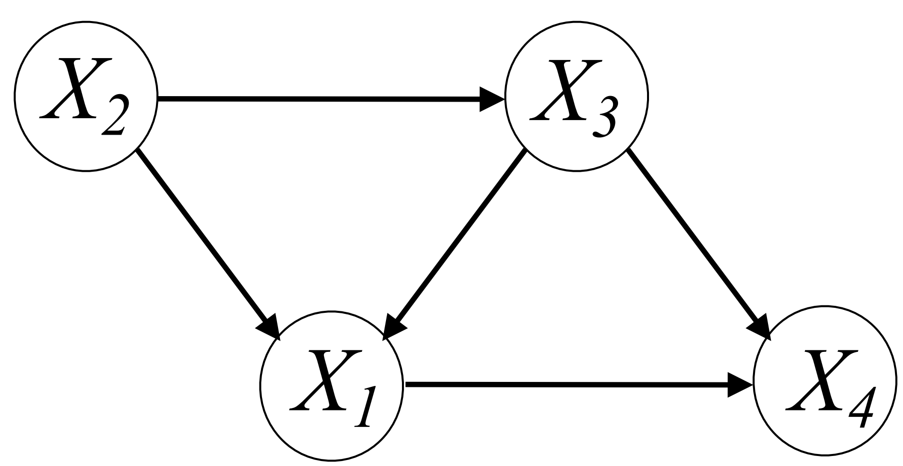
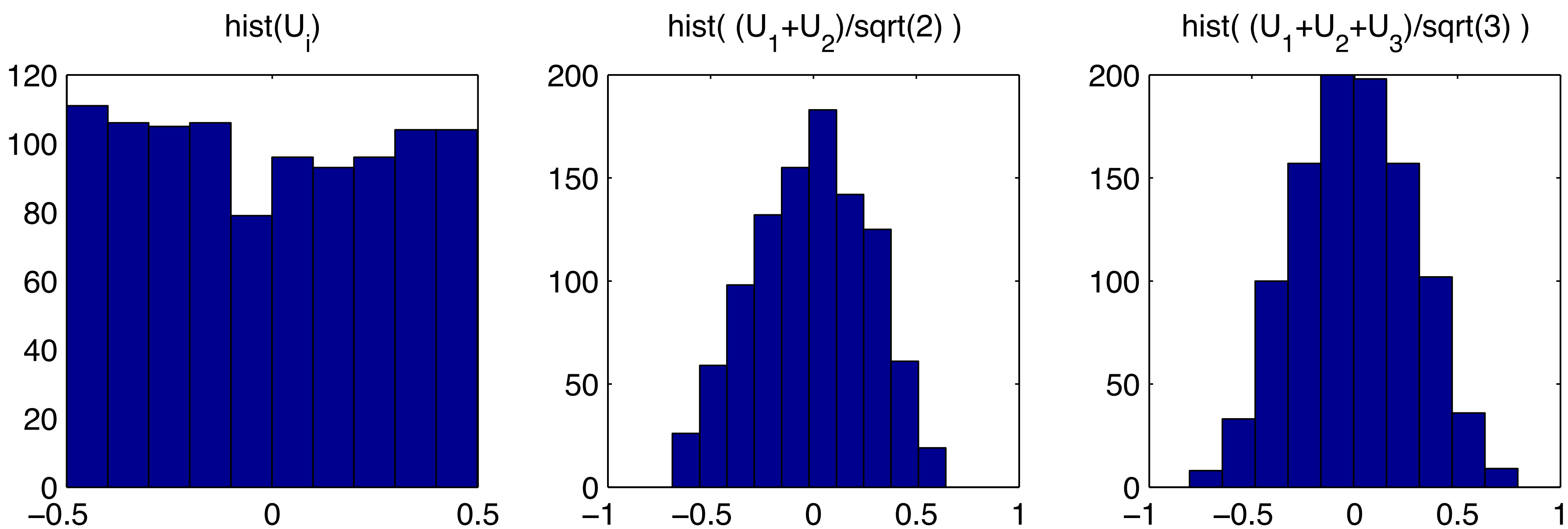


Why Gaussianity Was Widely Used?

- Central limit theorem: An illustration



- "Simplicity" of the form; completely characterized by mean and covariance

- Marginal and conditionals are also Gaussian

- Has maximum entropy, given values of the mean and the covariance matrix

E. T. Jaynes. Probability Theory: The Logic of Science. 1994. Chapter 7.

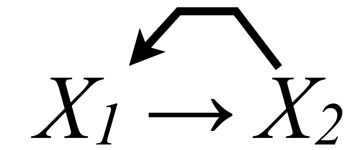
Gaussianity or Non-Gaussianity?

- Non-Gaussianity is actually ubiquitous
    - Linear closure property of Gaussian distribution: If the sum of any finite independent variables is Gaussian, then all summands must be Gaussian (Cramér, 1936)
    - Gaussian distribution is "special" in the linear case
- Practical issue: How non-Gaussian they are?

Practical Issues in Causal Discovery...

- Cycles (Richardson 1996; Lacerda et al., 2008)
- Nonlinearities (Zhang & Chan, ICONIP'06; Hoyer et al., NIPS'08; Zhang & Hyvärinen, UAI'09; Huang et al., KDD'18)
- Confounding (SGS 1993; Zhang et al., 2018c; Cai et al., NIPS'19; Ding et al., NIPS'19; Xie et al., NeurIPS'20); latent causal representation learning (Xie et al., NeurIPS'20; Cai et al., NeurIPS'19)
- Measurement error (Zhang et al., UAI'18; PSA'18)
- Selection bias (Spirtes 1995; Zhang et al., UAI'16)
- Missing values (Tu et al., AISTATS'19)
- Categorical variables or mixed cases (Huang et al., KDD'18; Cai et al., NIPS'18)
- Causality in time series
  - Time-delayed + instantaneous relations (Hyvarinen ICML'08; Zhang et al., ECML'09; Hyvarinen et al., JMLR'10)
  - Subsampling / temporally aggregation (Danks & Plis, NIPS WS'14; Gong et al., ICML'15 & UAI'17)
  - From partially observable time series (Geiger et al., ICML'15)
- Nonstationary/heterogeneous data (Zhang et al., IJCAI'17; Huang et al, ICDM'17, Ghassami et al., NIPS'18; Huang et al., ICML'19 & NIPS'19; Huang et al., JMLR'20)

Issue I: Feedback

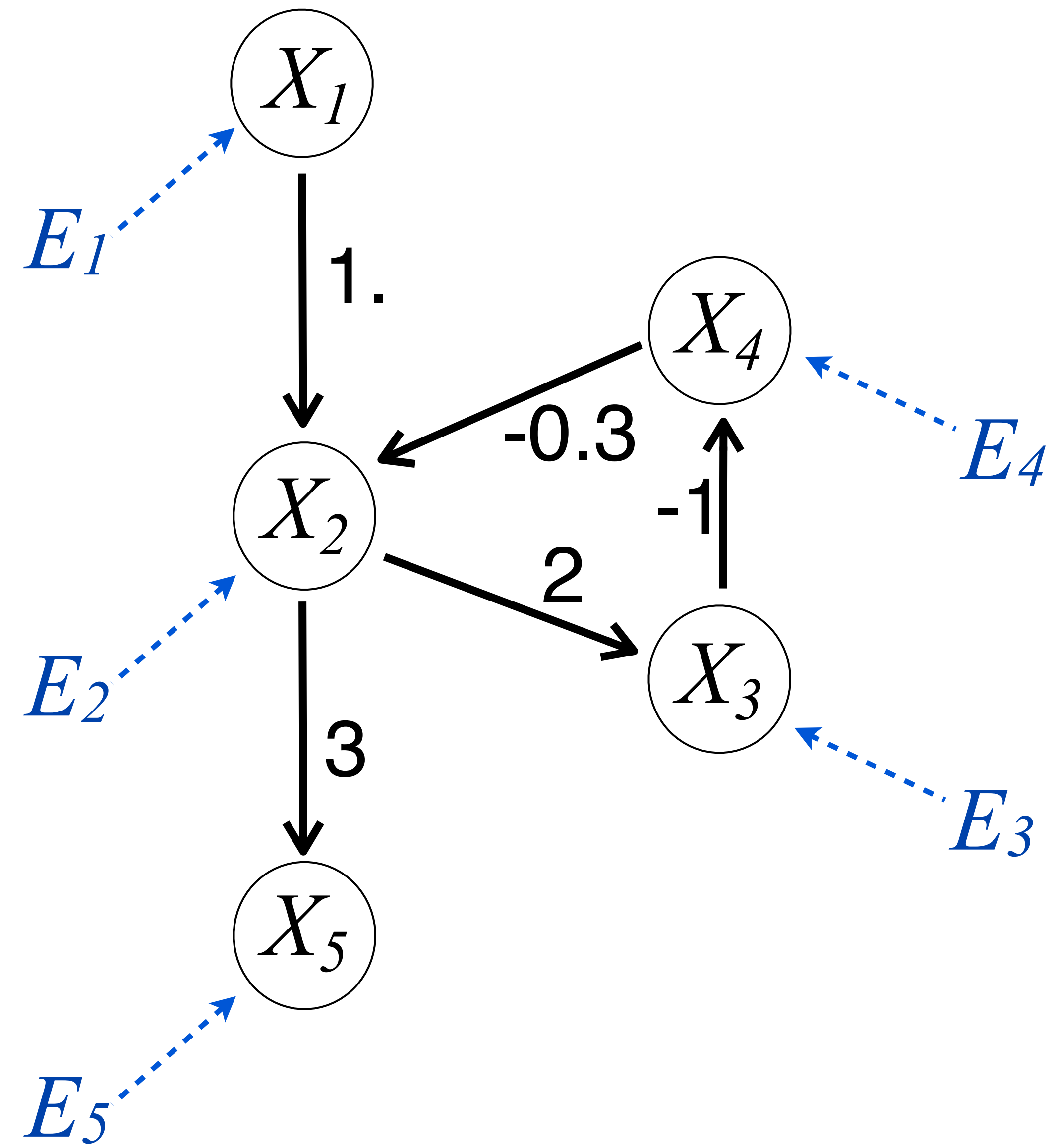


- Causal relations may have cycles; Consider an example

$$
\begin{aligned}
X_1 &= E_1 \\
X_2 &= 1.2X_1 - 0.3X_4 + E_2 \\
X_3 &= 2X_2 + E_3 \\
X_4 &= -X_3 + E_4 \\
X_5 &= 3X_2 + E_5
\end{aligned}
$$

Or in matrix form, $\mathbf{X} = \mathbf{B}\mathbf{X} + \mathbf{E}$, where

$$
\mathbf{B} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 1.2 & 0 & 0 & -0.3 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \end{bmatrix}
$$



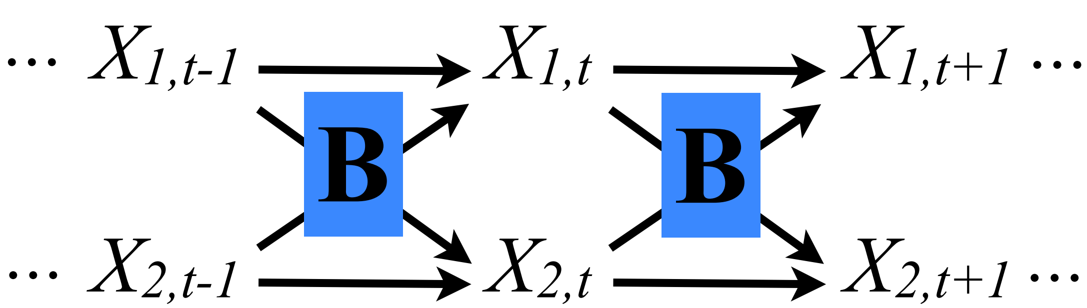
Lacerda, Spirtes, Ramsey and Hoyer (2008). Discovering cyclic causal models by independent component analysis. In Proc. UAI.

A conditional-independence-based method is given in T. Richardson (1996) - A Polynomial-Time Algorithm for Deciding Markov Equivalence of Directed Cyclic Graphical Models. Proc. UAI

Why Feedbacks?

$$\begin{tikzcd} X_1 \arrow[r] & X_2 \arrow[l, bend right] \end{tikzcd}$$

- Some situations where we can recover cycles with ICA:
  - Each process reaches its equilibrium state & we observe the equilibrium states of multiple processes



$$\mathbf{X}_t = \mathbf{B}\mathbf{X}_{t-1} + \mathbf{E}_t.$$

At convergence we have $X_t = X_{t-1}$ for each dynamical process, so

$$\mathbf{X}_t = \mathbf{B}\mathbf{X}_t + \mathbf{E}_t, \quad \text{or} \quad \mathbf{E}_t = (\mathbf{I} - \mathbf{B})\mathbf{X}_t.$$

  - On temporally aggregated data

Suppose the underlying process is $\tilde{\mathbf{X}}_t = \mathbf{B}\tilde{\mathbf{X}}_{t-1} + \tilde{\mathbf{E}}_t$, but we just observe $\mathbf{X}_t = \frac{1}{L}\sum_{k=1}^{L}\tilde{\mathbf{X}}_{t+k}$. Since

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We have $\mathbf{X}_t = \mathbf{B}\mathbf{X}_t + \mathbf{E}_t$ as $L \to \infty$.

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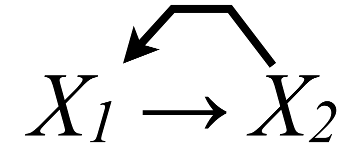

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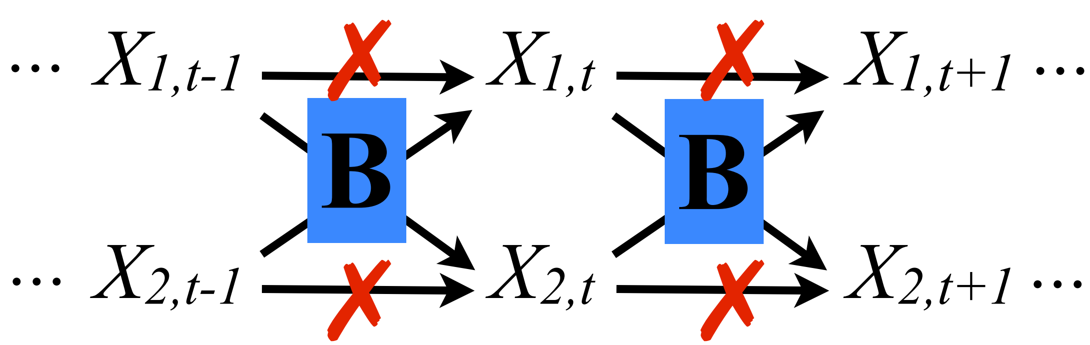

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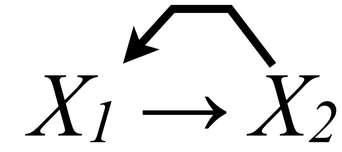
Examples



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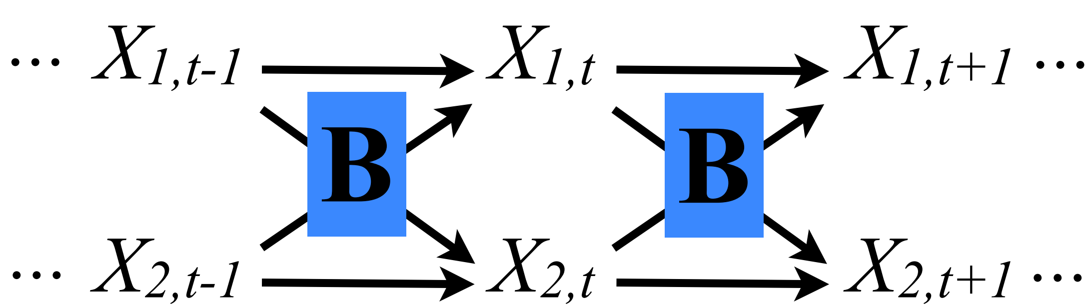

Consider the price and demand of the same product in different states:

$$\text{price}_t = b_1 \cdot \text{price}_{t-1} + b_2 \cdot \text{demand}_{t-1} + E_1$$
$$\text{demand}_t = b_3 \cdot \text{price}_{t-1} + b_4 \cdot \text{demand}_{t-1} + E_2$$

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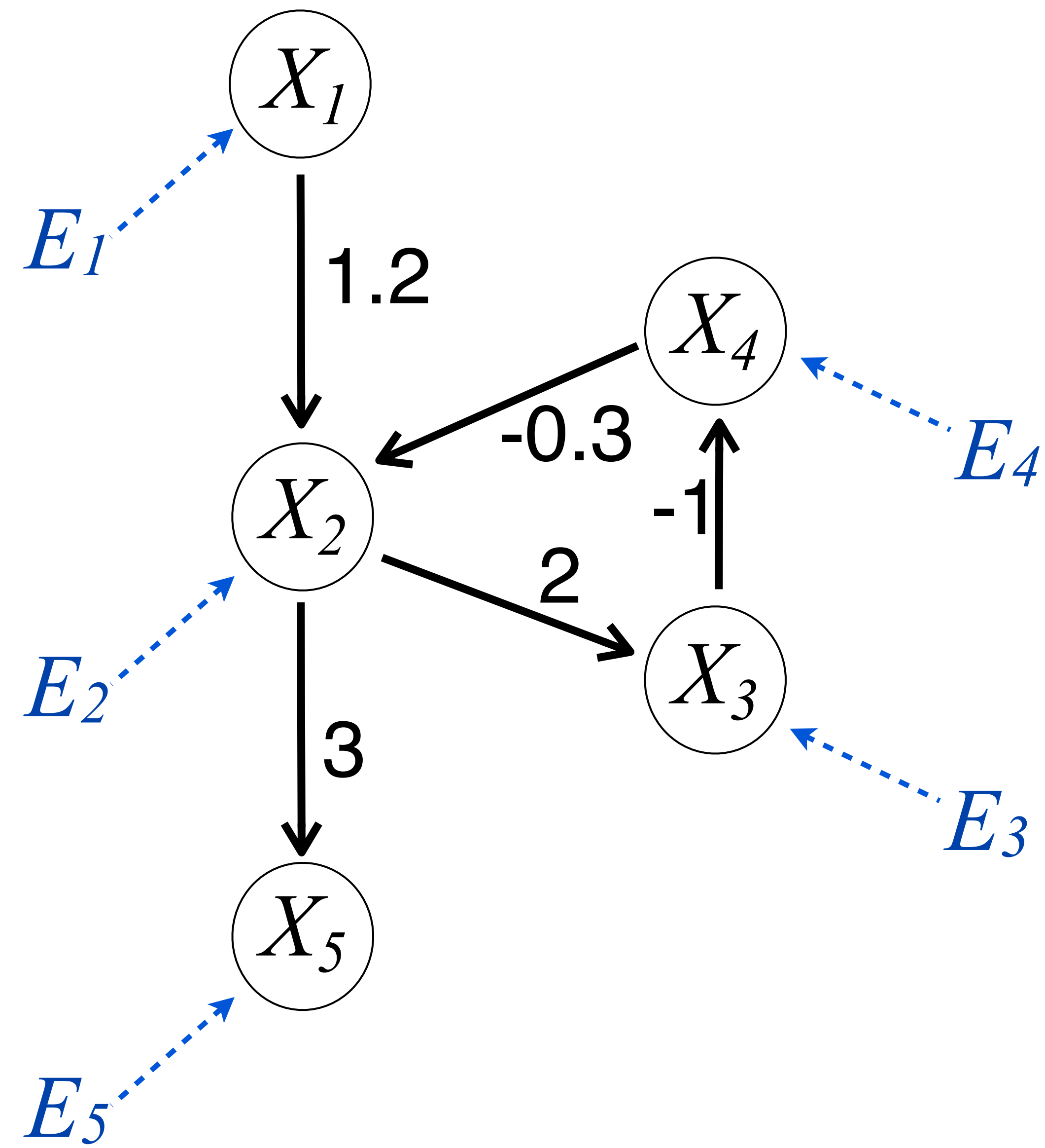
Consider the causal relation between two stocks: the causal influence takes place very quickly ($\sim$ 1-2 minutes) but we only have daily returns.

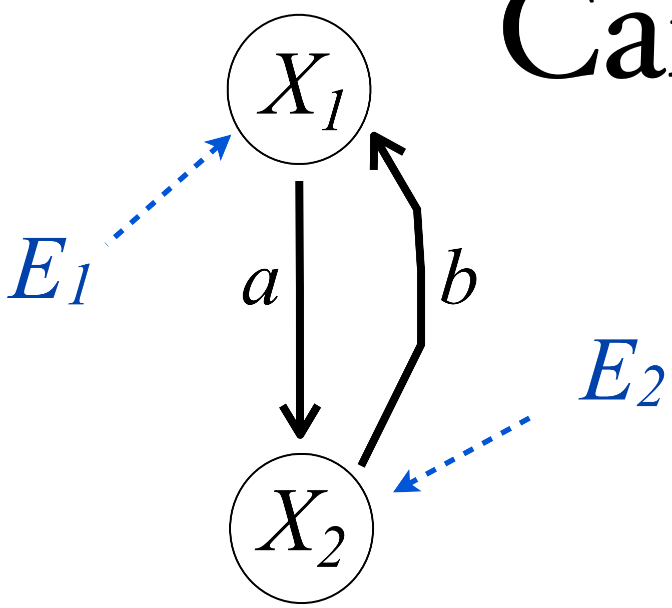
Cyclic Model: Global or Local Markov Condition?

- Local Markov condition?
- Global Markov condition?
  - Linear case?
  - General nonlinear case?



P. Spirtes, Directed Cyclic Graphical Representations of Feedback Models, UAI 1995

Can We Recover Cyclic Relations?



Suppose we have the process

$$\mathbf{X}_t = \underbrace{\begin{bmatrix} 0 & b \\ a & 0 \end{bmatrix}}_{\mathbf{B}} \mathbf{X}_t + \mathbf{E}_t.$$

That is,

$$(\mathbf{I}-\mathbf{B})\mathbf{X} = \mathbf{E}, \quad \text{or} \quad \underbrace{\begin{bmatrix} 1 & -b \\ -a & 1 \end{bmatrix}}_{\mathbf{W}} \mathbf{X}_t = \mathbf{E}_t$$

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- **E = (I-B)X**; ICA gives **Y = WX**
- Without cycles: unique solution to **B**
- With cycles: solutions to **B** not unique any more; why? :-(
  - A 2-D example?
- Only one solution is stable (assuming no self-loops), i.e., s.t. |*product of coefficients over the cycle*| < 1 :-)

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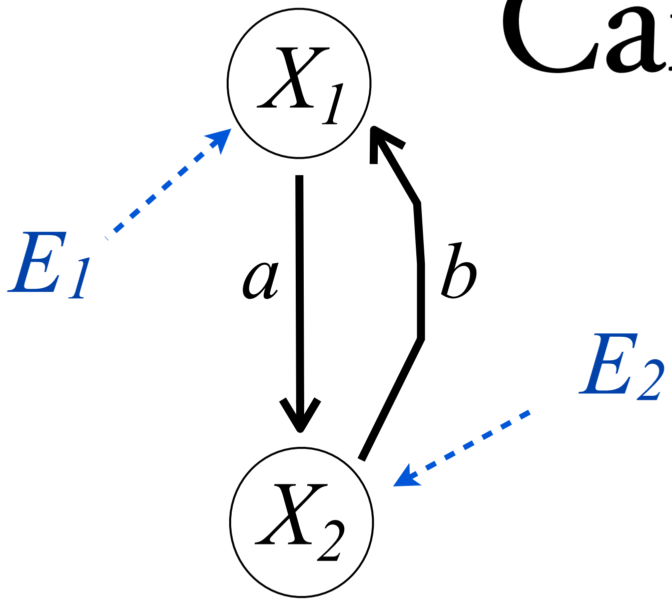

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Summary:

1. Still *m* independent components;
2. **W** cannot be permuted to be lower-triangular

Summary: LiNGAM

- We started making use of additional (plausible?) assumptions about causal mechanisms
  - Linear models with non-Gaussian noise
- Methods for estimating linear non-Gaussian causal models
- Difference between Linear, non-Gaussian and linear-Gaussian models
- Next: Interpretation and estimation of cyclic models