

構造方程式モデリングによる 因果構造探索

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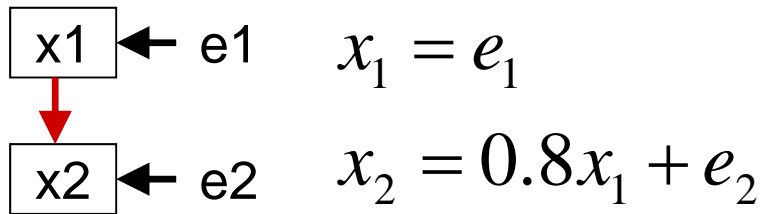
Abstract

- Linear structural equation models (SEMs) often used to represent data generating processes of continuous variables
- Conventional methods based on conditional independences or Gaussianity cannot identify a number of data generating models
- Non-Gaussian methods can identify many more data generating models

Motivation

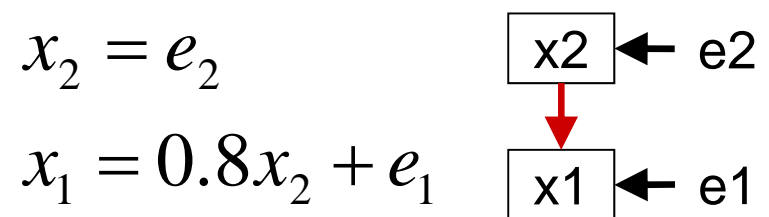
- Suppose that two observed variables x_1 and x_2 are linear mixtures of two independent latent variables e_1 and e_2
- You know that the mixing model (the data generating process) is either of the following two models (SEMs):

Model 1



or

Model 2



- You want to estimate which SEM is the actual data generating process based on a random sample X from $p(x_1, x_2)$

Motivation (continued)

- Conventional methods cannot do this
 - Because they only use conditional independence relations between x_1 and x_2 or assume **Gaussianity** (even if data is non-Gaussian)
- **Non-Gaussian** data is encountered in many applications:
 - Neuroinformatics (Hyvarinen et al., 2001); Bioinformatics (Sogawa et al., 2010); Social sciences (Micceri, 1989); Economics (Moneta et al., 2010)
- A new approach: **Non-Gaussian** approach
 - Non-Gaussianity allows to identify the data generating process: which of the two SEMs generated the data

Background:

Structural equation models (SEMs)

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Structural equation models

(Bollen, 1989; Pearl, 2000)

- Structural equation models (SEMs) integrate many multivariate statistical models
 - path analysis, factor analysis, autoregressive models, analysis of variance etc.
- SEMs can be used to represent **data generating processes**
- SEMs can be used to represent **causal relations** under some additional assumptions including a definition of causal effect

Background:

Structural equation models

(Bollen, 1989; Pearl, 2000)

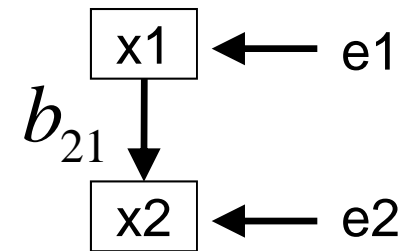
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A SEM represent a data generating process: Example

- A linear SEM (Bentler & Weeks, 1983)

$$x_1 = e_1$$

$$x_2 = b_{21}x_1 + e_2$$



- The SEM reads:
 - The value of x_1 is determined by that of e_1
 - The value of x_2 is determined by that of $x_1 (=e_1)$ and that of e_2

The latent variables e_1 and e_2 are called exogenous variables

(Bollen, 1989)

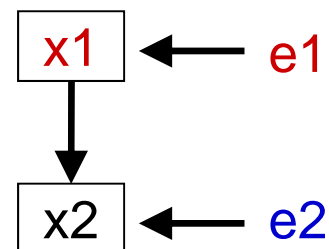
- An **exogenous variable** is a variable that is determined outside of the model: e_1 and e_2
- Two kinds of exogenous variables:
 1. Exogenous **observed** variables: $x_1=e_1$
 2. (latent) Disturbances: e_2

Structural equations:

$$x_1 = e_1$$

$$x_2 = b_{21}x_1 + e_2$$

Graph:



Basic linear SEM: DAG-SEM

(Bollen 1989)

- A linear acyclic SEM with independent exogenous variables:
 - Graphically represented by a directed acyclic graph (**DAG**)
 - Observed random vector \mathbf{x} is **linearly** modeled by

$$x_i = \sum_{j \neq i} b_{ij} x_j + e_i \quad \text{or} \quad \mathbf{x} = \mathbf{B}\mathbf{x} + \mathbf{e}$$

where

- The e_i are **exogenous variables** with non-zero variance and are mutually **independent**
- The ‘path-coefficient’ matrix | $\mathbf{B} = [b_{ij}]$ is constant
- **Acyclicity**

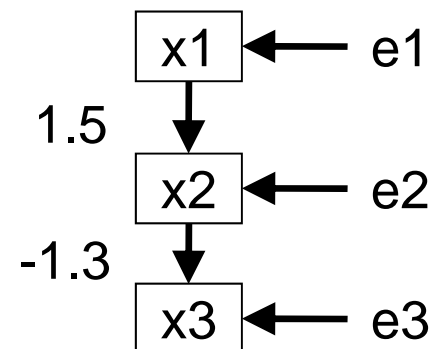
Example

- Structural equations:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 1.5 & 0 & 0 \\ 0 & -1.3 & 0 \end{bmatrix}}_{\mathbf{B}} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix}$$

- Associated DAG:

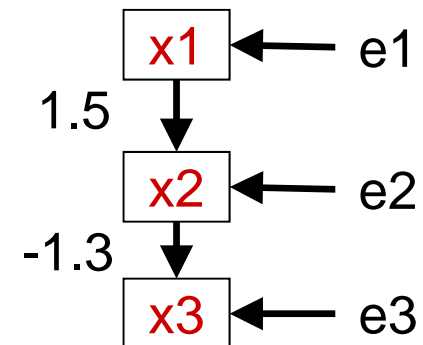
- x1 is a **parent** of x2
- x1 is an **ancestor** of x3
- x2 is a **child** of x1
- x3 is a **descendant** of x1



Assumption of acyclicity

- **Acyclicity** ensures existence of an ordering of variables x_i that permutes **matrix B** lower-triangular with zeros on the diagonal
- In the example, the ordering is $x_1 < x_2 < x_3$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 1.5 & 0 & 0 \\ 0 & -1.3 & 0 \end{bmatrix}}_{\mathbf{B}} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix}$$



Dependent exogenous variables result from latent variables

- A latent variable (**confounder**) f_1 introduces dependency between e_1 and e_2 :

$$x_1 = e_1$$

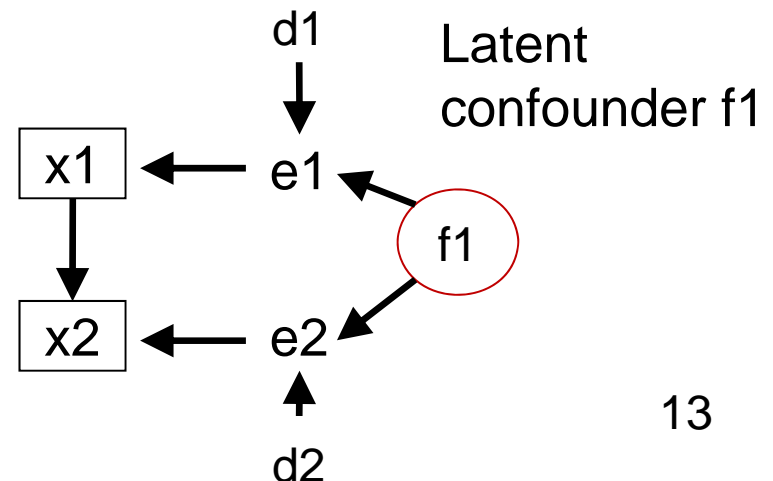
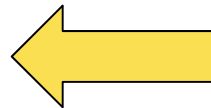
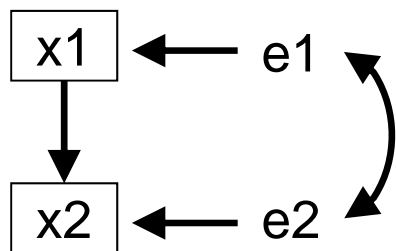
$$x_2 = 3x_1 + e_2$$

+

$$e_1 = 2f_1 + d_1$$

$$e_2 = 3f_1 + d_2$$

- Associated graphs



Background:

Structural equation models

(Bollen, 1989; Pearl, 2000)

- Structural equation models (SEMs) integrate many multivariate statistical models
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- SEMs can be used to represent **data generating processes**
- SEMs can be used to represent **causal relations** under some additional assumptions including a definition of causal effect

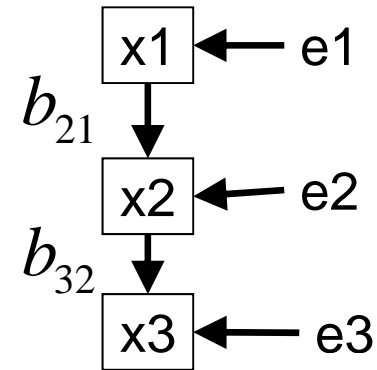
Can give a causal meaning to each path-coefficient b_{ij} (Pearl, 2000)

- Example:

$$x_1 = e_1$$

$$x_2 = b_{21}x_1 + e_2$$

$$x_3 = b_{32}x_2 + e_3$$



- Causal meaning of b_{32} :

- If you **change** x_2 from c_0 to c_1 , then $E(x_3)$ will **change** by $b_{32}(c_1 - c_0)$

'Change x2 from c0 to c1'

- It means 'Fix x2 at c0 regardless of the variables that previously determined x2 (do(x2=c0)) and change the constant from c0 to c1' (Pearl, 2000)
- In the SEM, **'Replace** the function determining x2 with a constant c0':

$$\begin{array}{l} x_1 = e_1 \\ x_2 = b_{21}x_1 + e_2 \\ \hline x_3 = b_{32}x_2 + e_3 \end{array}$$



Mutilated model
with do(x2=c0):

$$\begin{array}{l} x_1 = e_1 \\ x_2 = c_0 \\ \hline x_3 = b_{32}x_2 + e_3 \end{array}$$

(Assumption of invariance: the other functions don't change)

Average causal effect: Definition (Rubin, 1973; Pearl, 2000)

- Average causal effect of x_2 on x_3 when changing x_2 from c_0 to c_1 :

$$\begin{aligned} & E(x_3 \mid do(x_2 = c_1)) - E(x_3 \mid do(x_2 = c_0)) \\ &= b_{32}(c_1 - c_0) \end{aligned}$$

Computed based on the mutilated models with $do(x_2=c_1)$ or $do(x_2=c_0)$

- Causal meaning of b_{32} :
 - If you **change** x_2 from c_0 to c_1 , then $E(x_3)$ will **change** by $b_{32}(c_1 - c_0)$

Conducting experiments with random assignment is a method to estimate average causal effects

- Random assignment of participants into two groups:
 - Experimental group with $x_2 = c_1$
 - Control group with $x_2 = c_0$
- This fixes x_2 to c_1 or c_0 regardless of the variables that determines x_2

$$E(x_3 | do(x_2 = c_1)) - E(x_3 | do(x_2 = c_0))$$

$E(x_3)$ for the exp. group - $E(x_3)$ for the control group

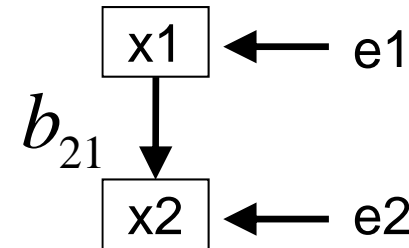
Estimate average causal effects using non-experimental data

- Experiments with random assignment often difficult to conduct: costs, ethics, etc.
- Sometimes, average causal effects can be estimated using non-experimental data (Pearl, 2000; Spirtes et al., 2000)
- Non-Gaussian methods presented in this tutorial can be used to estimate average causal effects based on non-experimental data

Basic problem setup: Learning DAG-SEMs

- Assume that data X is randomly sampled from a DAG-SEM (linear, acyclic, no latent confounder):

$$\mathbf{x} = \mathbf{B}\mathbf{x} + \mathbf{e}$$



- Goal: Estimate the path-coefficient matrix \mathbf{B} observing data X only!
 - Understand the data generating process
 - Compute average causal effects

Structural equation models (SEMs): Summary

- SEMs can be used to represent data generating processes
- If you **accept** that all the model assumptions are reasonable in your data, you **can analyze** the data generating process
- If you further **accept** the definition of causal effect, you **can analyze** causal relations
- SEMs help you to elaborate your theory
- Basic model is DAG-SEM
 - Various extensions extensively discussed

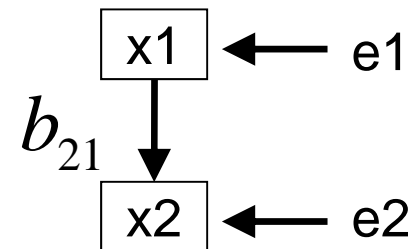
Problems:
**Identifiability problems of
conventional methods**

Under what conditions B is identifiable?

- Identifiable = uniquely determined or estimated from $p(x)$

- DAG-SEM:

$$\mathbf{x} = \mathbf{B}\mathbf{x} + \mathbf{e}$$



- B and $p(e)$ induce $p(x)$
- If $p(x)$ are different for different B , then B is uniquely estimated

Conventional estimation principle: Causal Markov condition

- If the data generating model is a DAG-SEM, causal Markov condition holds :
 - Each observed variable x_i is **independent** of its non-descendants in the DAG **conditional** on its parents (Pearl & Verma, 1991) :

$$p(\mathbf{x}) = \prod_{i=1}^p p(x_i \mid \text{parents of } x_i)$$

Conventional methods based on causal Markov condition

- **Methods based on conditional independencies**
(Spirtes & Glymour, 1991)
 - Many DAG-SEMs give same set of conditional independences and equally fit data
- **Scoring methods based on Gaussianity**
(Chickering, 2002)
 - Many DAG-SEMs give the same Gaussian distribution and the same scores like BIC
- **Often path-coefficient matrix B is not uniquely determined or estimated**

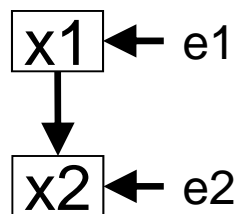
Example

- Two models with Gaussian e_1 and e_2 :

Model 1:

$$x_2 = 0.8x_1 + e_2$$

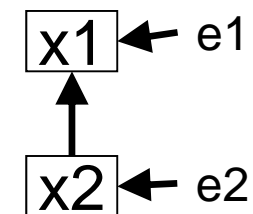
$$\mathbf{B} = \begin{bmatrix} 0 & 0 \\ 0.8 & 0 \end{bmatrix}$$



Model 2:

$$x_1 = 0.8x_2 + e_1$$

$$\mathbf{B} = \begin{bmatrix} 0 & 0.8 \\ 0 & 0 \end{bmatrix}$$



$$E(e_1)=E(e_2)=0, \text{var}(x_1) = \text{var}(x_2)=1$$

- Both introduce no conditional independence:

$$\text{cov}(x_1, x_2) = 0.8 \neq 0$$

- Both induce same Gaussian distribution:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \sim N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}\right)$$

A solution:
Non-Gaussian approach

A new direction: Non-Gaussian approach

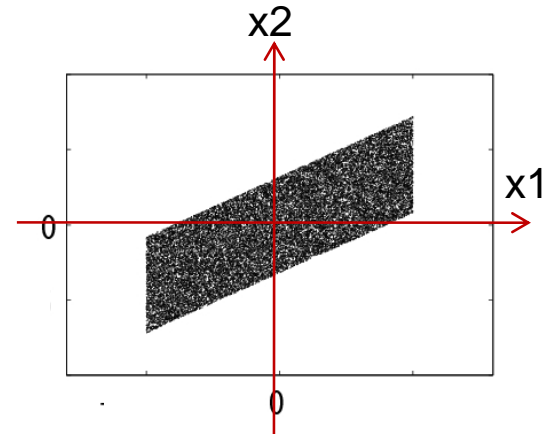
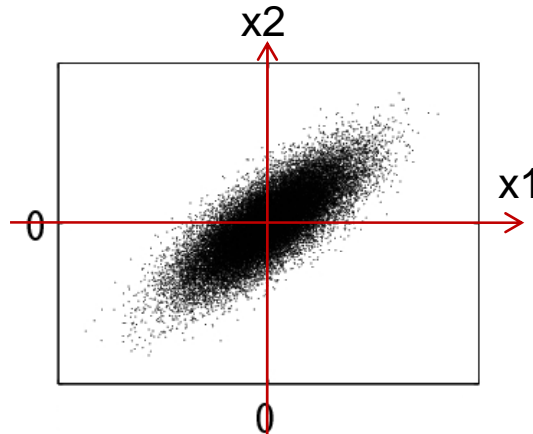
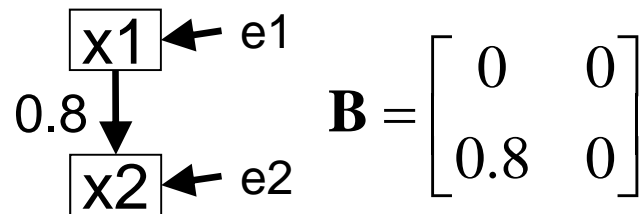
- Non-Gaussian data in many applications:
 - Neuroinformatics (Hyvarinen et al., 2001); Bioinformatics (Sogawa et al., 2010); Social sciences (Micceri, 1989); Economics (Moneta et al., 2010)
- Utilize non-Gaussianity for model identification (Bentler, 1983)
- The path-coefficient matrix **B** is uniquely estimated from $p(x)$ if e_i are non-Gaussian
 - (Shimizu, Hoyer, Hyvarinen & Kerminen, JMLR, 2006)

Illustrative example: Gaussian vs non-Gaussian

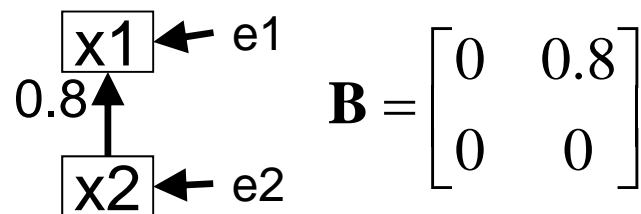
Gaussian

Non-Gaussian
(uniform)

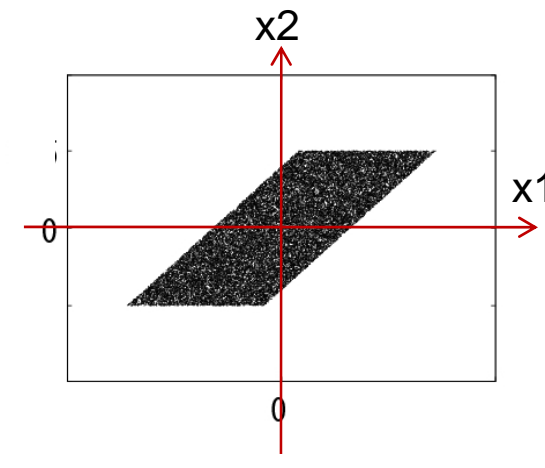
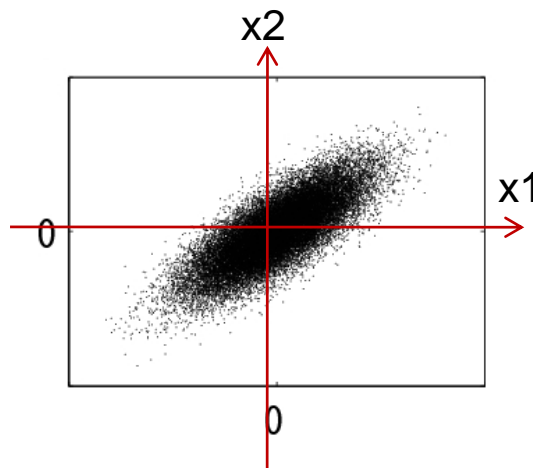
Model 1:



Model 2:



$E(e_1) = E(e_2) = 0$
 $\text{Var}(x_1) = \text{var}(x_2) = 1$



Linear Non-Gaussian Acyclic Model: LiNGAM

(Shimizu, Hyvarinen, Hoyer & Kerminen, JMLR, 2006)

- An **identifiable** non-Gaussian version of DAG-SEM:

$$x_i = \sum_{j \neq i} b_{ij} x_j + e_i \quad \text{or} \quad \mathbf{x} = \mathbf{B}\mathbf{x} + \mathbf{e}$$

where

– The e_i are

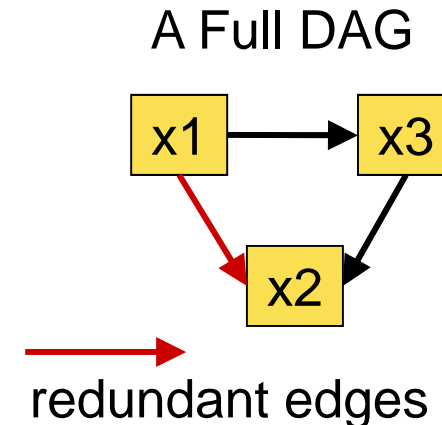
- exogenous variables with non-zero variance
- (non-degenerate) **non-Gaussian**
- mutually independent

– **Acyclicity**

Two estimation algorithms

- **LiNGAM algorithm**
(Shimizu, Hoyer, Hyvarinen & Kerminen, JMLR, 2006)
- **DirectLiNGAM algorithm**
(Shimizu, Hyvarinen, Kawahara & Washio, UAI09)
- Both estimates an ordering of variables that makes the path-coefficient matrix \mathbf{B} to be lower-triangular
 - Acyclicity ensures existence of such an ordering

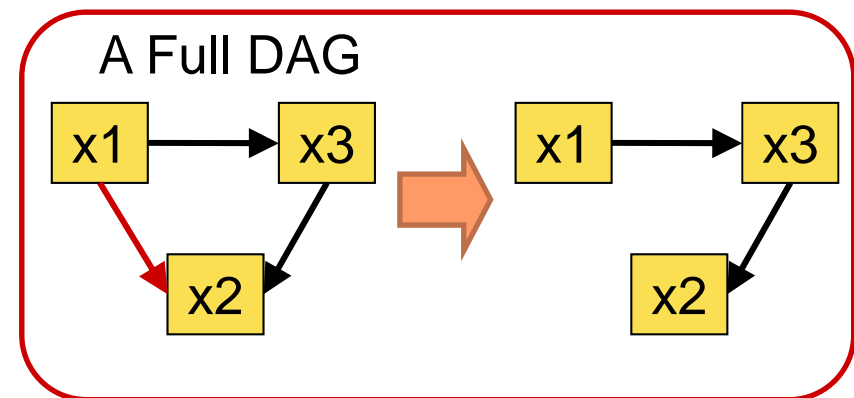
$$\mathbf{x}_{perm} = \underbrace{\begin{bmatrix} & & \mathbf{0} \\ & & \\ \mathbf{B}_{perm} & & \end{bmatrix}}_{\mathbf{B}_{perm}} \mathbf{x}_{perm} + \mathbf{e}_{perm}$$



Once such an ordering is found...

- Many existing methods can do:
 - Pruning the remaining path-coefficients
 - sparse methods like weighted lasso (Zou, 2006)
 - Finding significant path-coefficients
 - Testing, bootstrapping (Shimizu et al., 2006; Hyvarinen 2010)

$$\mathbf{x}_{perm} = \underbrace{\begin{bmatrix} * & & & \mathbf{0} \\ 0 & * & & \\ * & 0 & * & \\ * & 0 & * & \end{bmatrix}}_{\mathbf{B}_{perm}} \mathbf{x}_{perm} + \mathbf{e}_{perm}$$



まとめ

- Use of **non-Gaussianity** in linear SEMs is useful for **model identification**
- Non-Gaussian data encountered in many applications
- The non-Gaussian approach can be **a good option**
- Links to codes and papers:
<http://homepage.mac.com/shoheishimizu/lingampapers.html>