



# Discovering Cyclic Causal Models by Independent Components Analysis

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# Our goal

- Discover the structure and parameters of linear SEMs, without experimental data.

# Outline

- Linear SEMs
- LiNGAM method (*Shimizu et al 2006*): uniquely identifies acyclic linear SEMs, by using ICA
- LiNG-D: our new method, based on LiNGAM, but handles cycles
- Now, the answer given is underdetermined
- But we argue that stability can be a powerful constraint

# Linear SEMs

- Directed graphical models that represent **causal** relationships.

M:

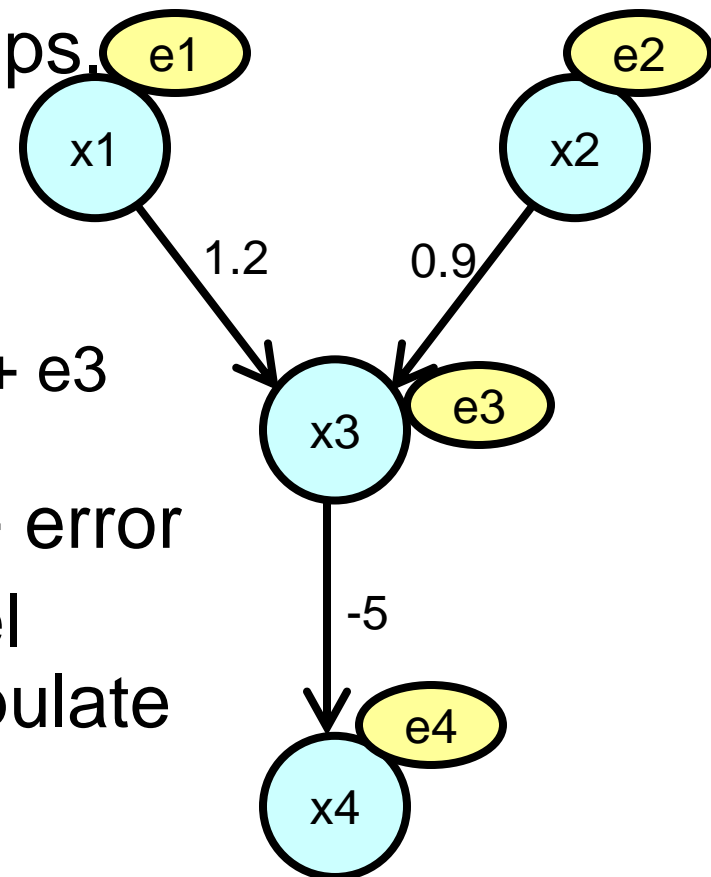
$$x_1 = e_1$$

$$x_2 = e_2$$

$$x_3 = 1.2 x_1 + 0.9 x_2 + e_3$$

$$x_4 = -5 x_3 + e_4$$

- linear combination of parents + error
- “causal” means that they model what happens when you manipulate
- e.g. manipulating  $x_3$ ...



# Linear SEMs

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$M(\text{do}(x_3=k)):$

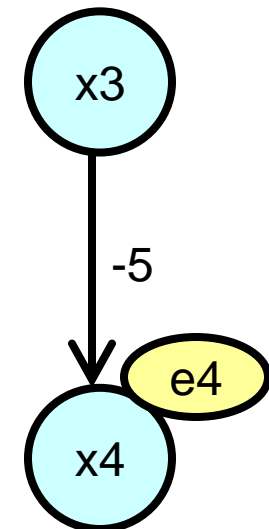
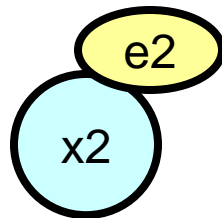
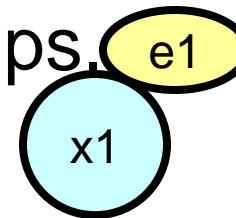
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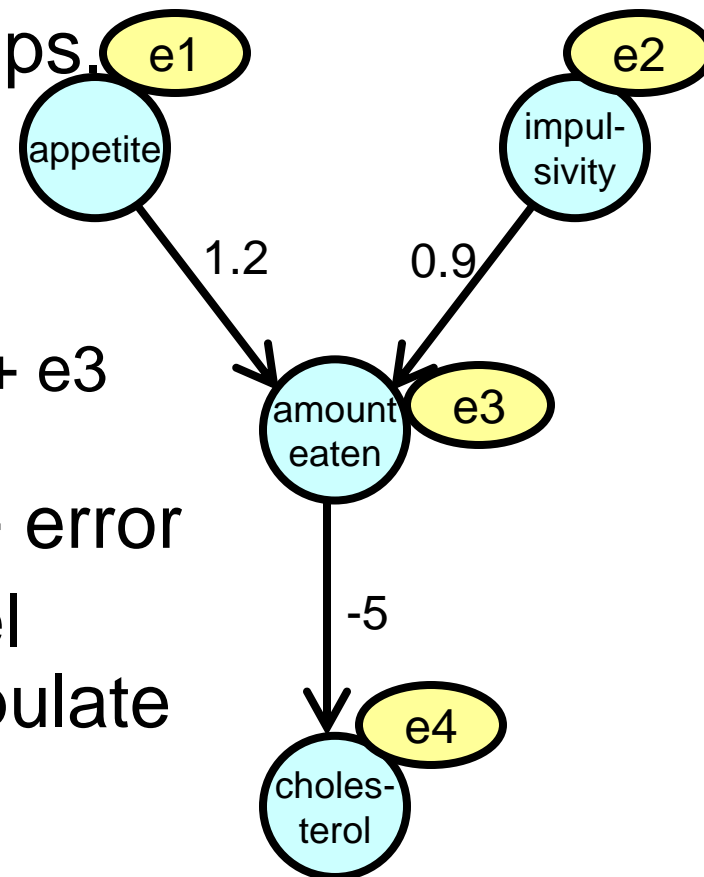
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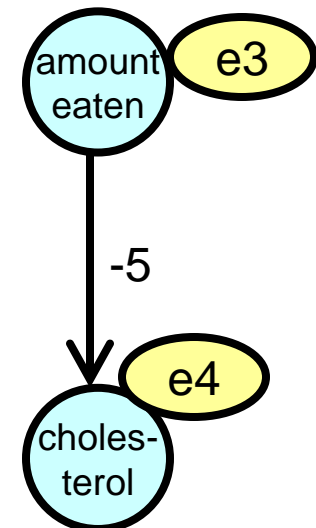
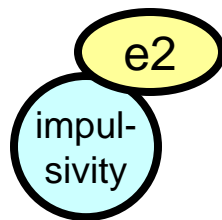
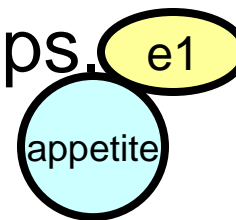
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# Linear SEMs can be cyclic too

- Correspond to dynamical systems:

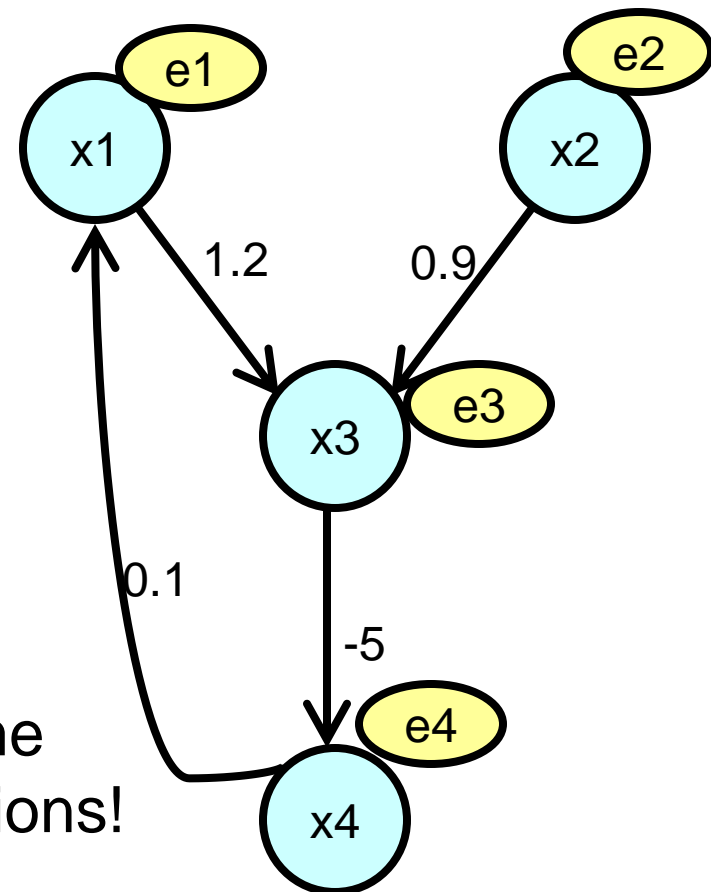
$$\mathbf{x3}[t+1] = 1.2 \mathbf{x1}[t] + 0.9 \mathbf{x2}[t] + \mathbf{e3}$$

etc.

- Deterministic
- Reach equilibria (unless unstable)

$$\mathbf{x3}_{eq} = 1.2 \mathbf{x1}_{eq} + 0.9 \mathbf{x2}_{eq} + \mathbf{e3}$$

- Equilibrium equations have the same coefficients as the dynamical equations!





# Our goal

- Given the equilibrium data  $\mathbf{x}$ , recover the structure of the process, i.e. values of  $B$  that entail the observed distribution of equilibria

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

# Linear SEMs

- **Claim:** joint distribution of  $\mathbf{e}$  + the equations  $\rightarrow$  joint distribution of  $\mathbf{x}$ .

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

- Solving for  $\mathbf{x}$ , we get:

$$\mathbf{x} = (\mathbf{I} - \mathbf{B})^{-1} \mathbf{e}$$

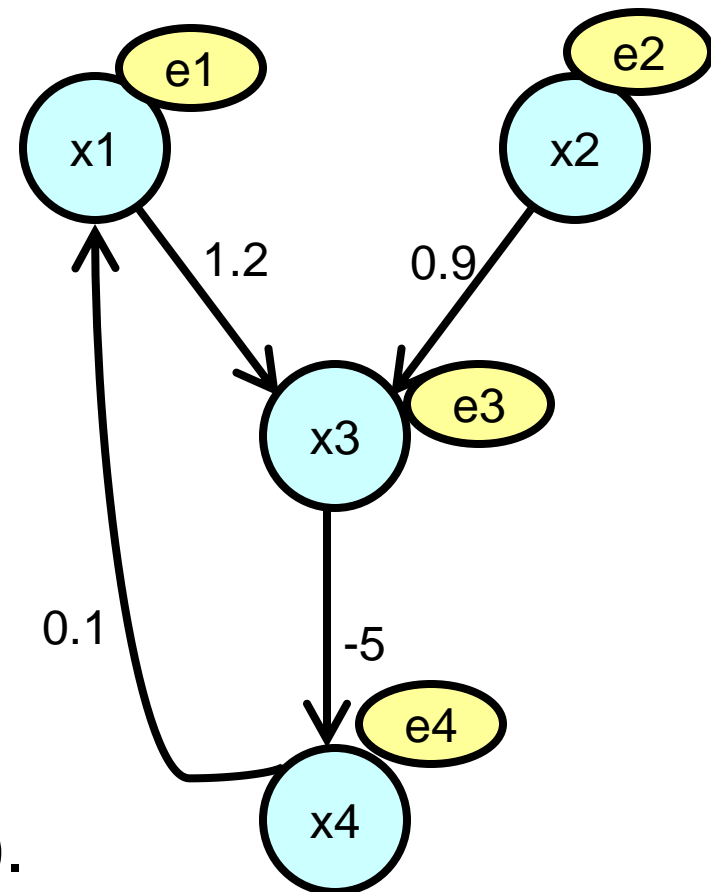
- QED.

- Cycles  $\rightarrow$  infinite sums

- Let  $\mathbf{A} = (\mathbf{I} - \mathbf{B})^{-1}$

$$\text{then } \mathbf{x} = \mathbf{A} \mathbf{e}$$

( $\mathbf{A}$  is called the “mixing matrix”).




# Our assumptions

- Data are equilibria of a linear SEM
- The sample data is i.i.d.
- The error terms have a positive variance
- At most one error term is Gaussian
- Weak Causal Markov: if  $X$ ,  $Y$  causally unconnected, then they are independent
- Causal sufficiency (no hidden confounders)
- “causal faithfulness”: the effect of  $e_i$  on  $x_i$  is not zero.

# Causal Faithfulness and violations

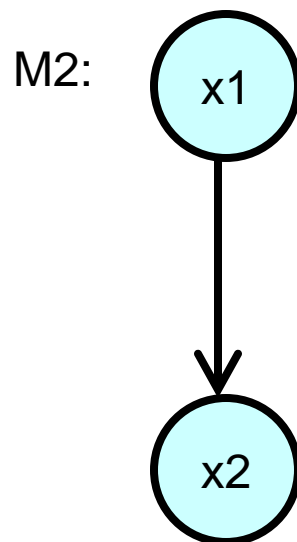
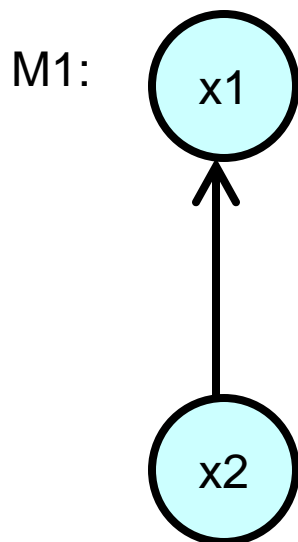
- **Definition:** In the equilibrium, the effect of  $e_i$  on  $x_i$  (reduced-form coefficient) is not 0.
- Acyclic case: never violated
- Cyclic case, violations:
  - e.g. 1:  $x_1[t+1] = 1 * x_1[t] + \dots$
  - e.g. 2: a polynomial function of the cycle-products of the SEMs is equal to 1

# Outline

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- LiNG-D: our new method, based on LiNGAM, but handles cycles
- Now,  $B$  is not unique
- But we show that stability can be a powerful constraint

# How much can be identified from observational data alone?

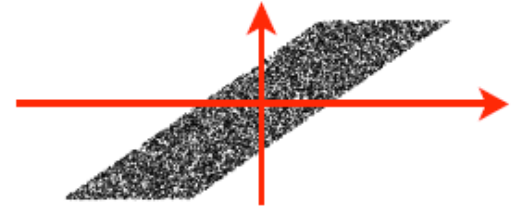
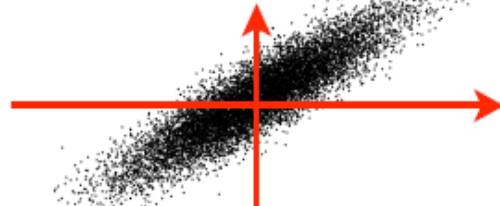
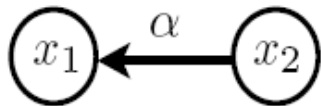
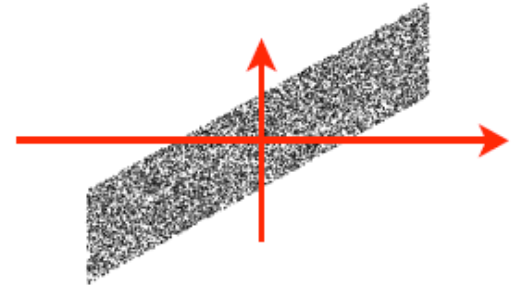
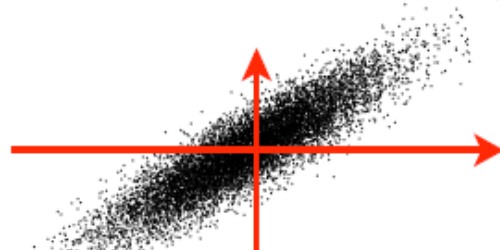
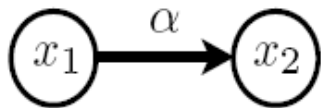
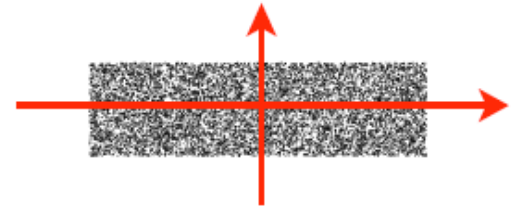
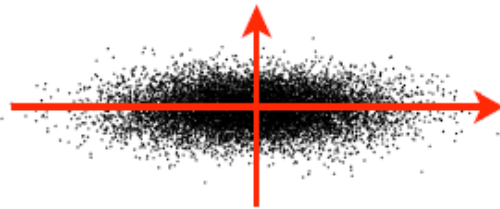
- When Gaussian, d-separation equivalence class
- e.g. can't tell the difference between:



# Why not?

Gaussian

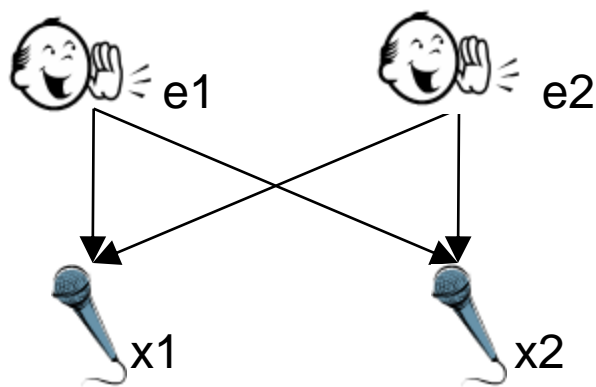
Uniform



Images by Patrik Hoyer et al, used with permission  
from "Estimation of causal effects using linear non-Gaussian causal models with hidden variables"

# Independent Components Analysis (ICA)

- Cocktail party problem



$$\mathbf{x} = \mathbf{A} \mathbf{e}$$

- You want to get back the original signals, i.e. we need the inverse of the mixing matrix

Let  $\mathbf{W} = \mathbf{A}^{-1}$   
Then  $\mathbf{e} = \mathbf{W} \mathbf{x}$   
and  $\mathbf{W} = \mathbf{I} - \mathbf{B}$

- in general case, there would be infinitely many solutions for  $\mathbf{A}$ .
- BUT, assuming independence and non-Gaussianity, it is possible to estimate  $\mathbf{A}$  and  $\mathbf{e}$  from just  $\mathbf{x}$ . This is what ICA does.





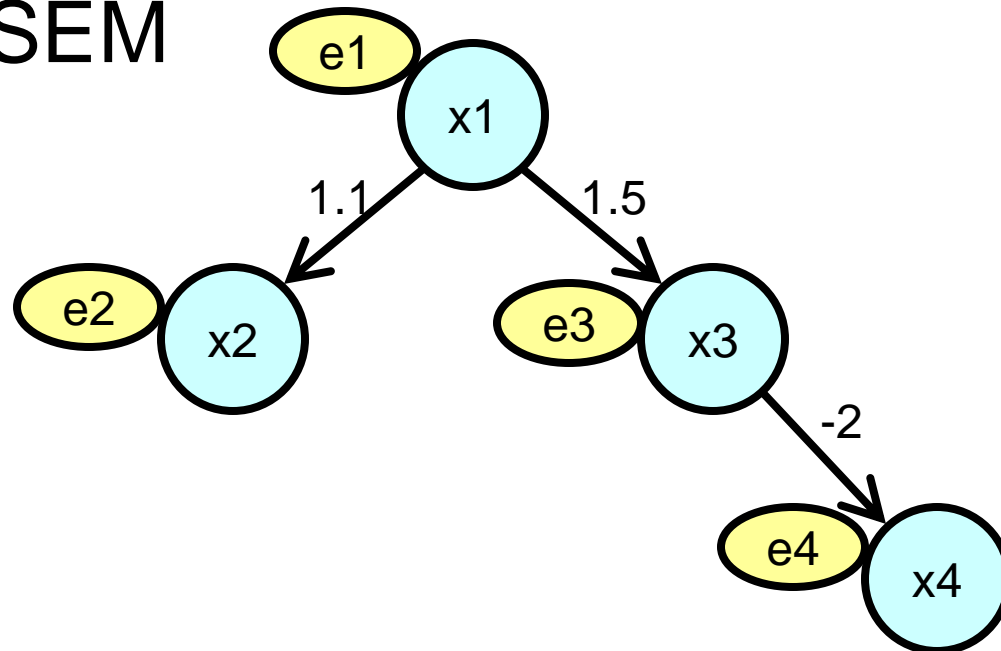
# Independent Components Analysis (ICA)

- sources in cocktail-party problem = error terms in SEMs
- Underdetermination: ICA returns  $W$  up permutation of error terms

# The LiNGAM method

*(Shimizu et al, 2006)*

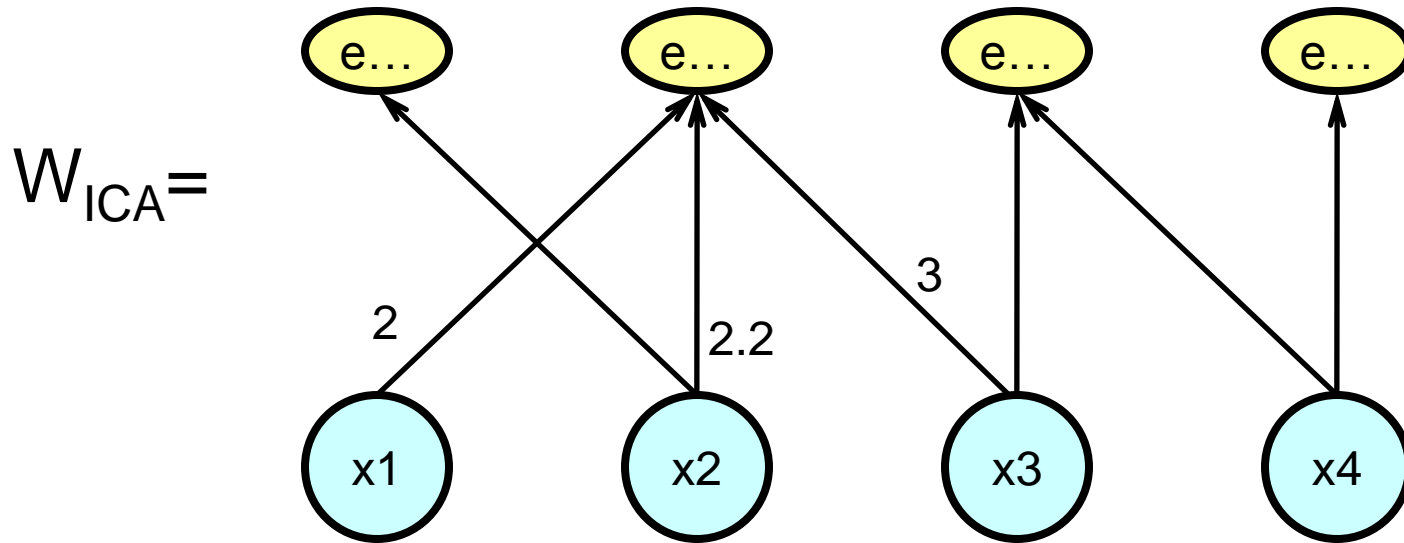
- What happens if we generate data from this linear SEM



- ... and then run ICA?

# The LiNGAM method

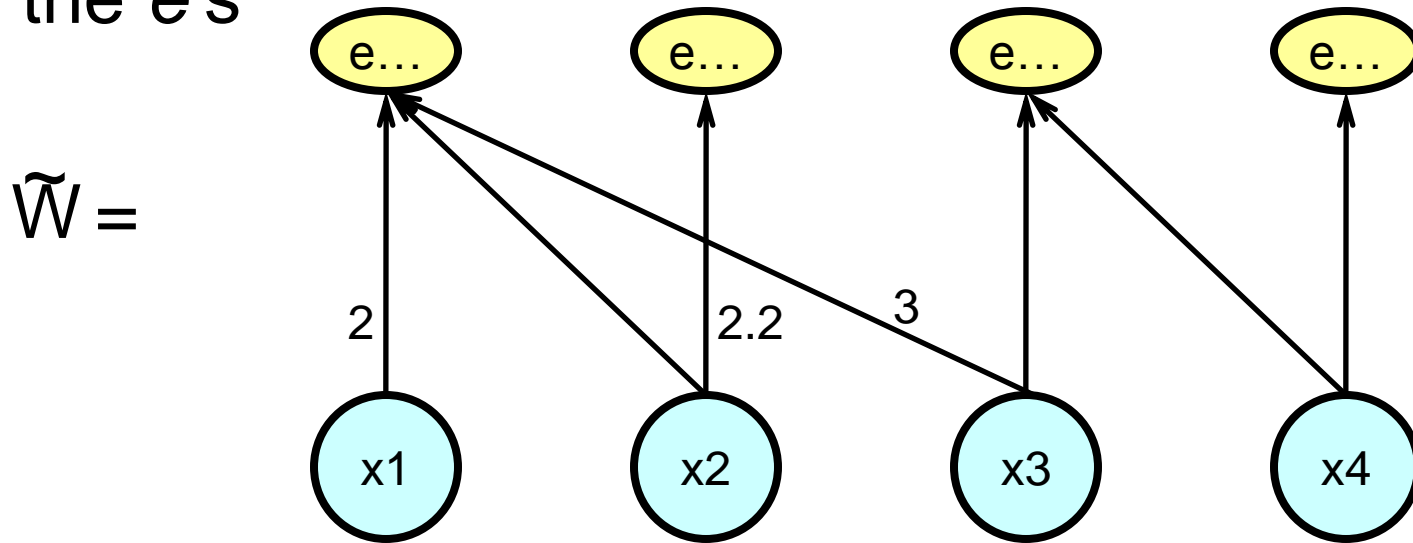
- ICA returns a  $W$  matrix such as:



- So **first** we need to find the right permutation of the e's

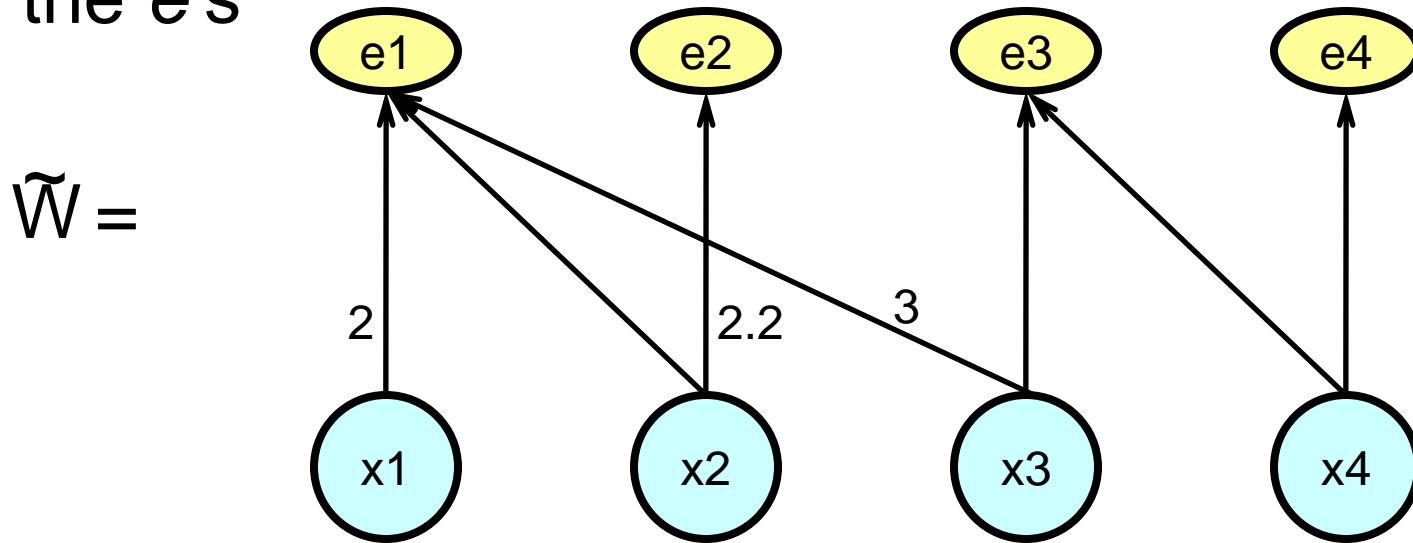
# The LiNGAM method

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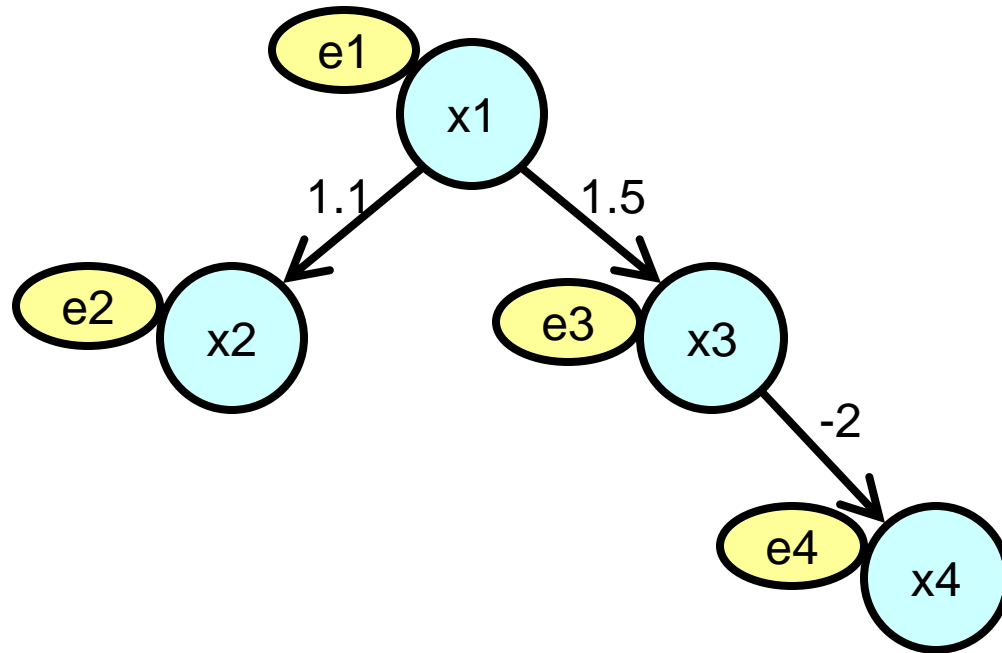


- We label the  $e$ 's accordingly

# The LiNGAM method

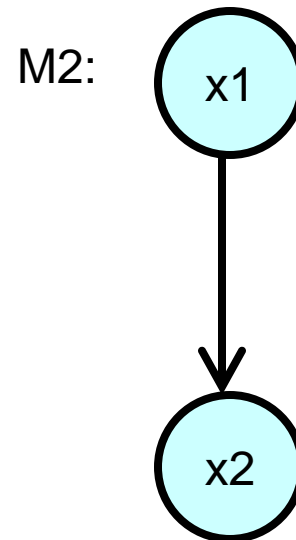
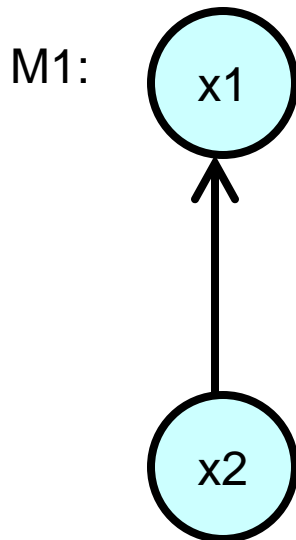
- Using the equation  $B = I - W'$ , we get back:

B =

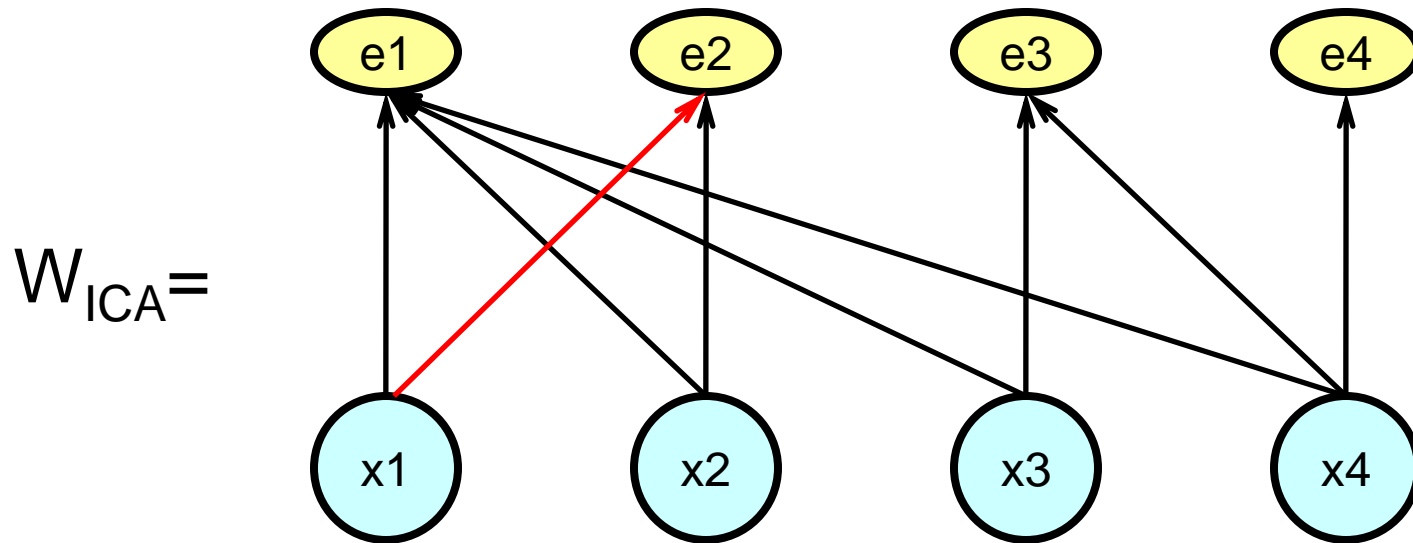


# The LiNGAM method

- Discovers the full structure of the DAG
  - causal sufficiency  $\leftrightarrow$  independence of the error terms
- In particular, now M1 and M2 can be distinguished!



# The LiNGAM method – limitation





# The LiNGAM method – limitation

- LiNGAM cannot discover cyclic models...
- because:
  - since it assumes the data was generated by a DAG,
  - it searches for a single valid permutation, by searching for an ordering
- If we stop imposing an ordering, and search for any number of valid permutations...
- then we can discover cyclic models too.
- That's exactly what we did!



# The LiNG-D method

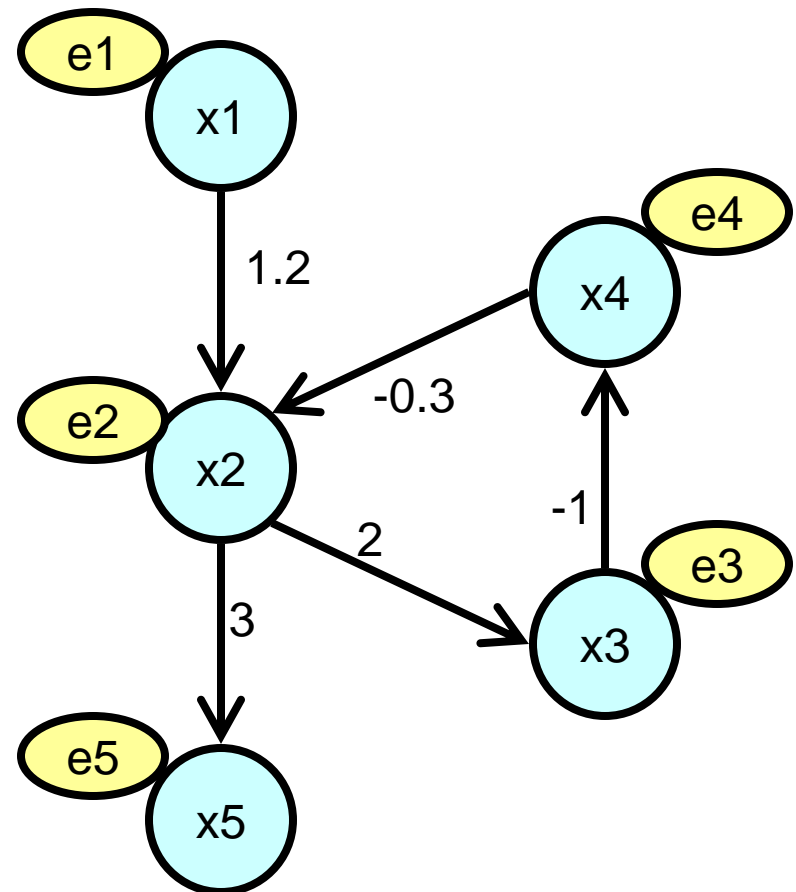
- When the data looks acyclic, it works just like LiNGAM, and returns a single model.
- When the data looks cyclic, more than one permutation is considered valid. Thus, it returns a distribution-equivalent set containing more than one model.
- “distribution-equivalent” means you can’t do better, at least without experimental data or further assumptions.

# The LiNG-D method

- Finds (multiple) row-permutations of  $W_{ICA}$  that have no zeros in the diagonal
- equivalent to Constrained n-Rooks Problem
- Naïve algorithm: depth-first search
- Better algorithm: set all zeros to 0, all nonzeros to 1, and run  $k$ -th best assignments algorithm (linear programming) until get a score less than  $n$ .
- Worst case:  $n!$  models

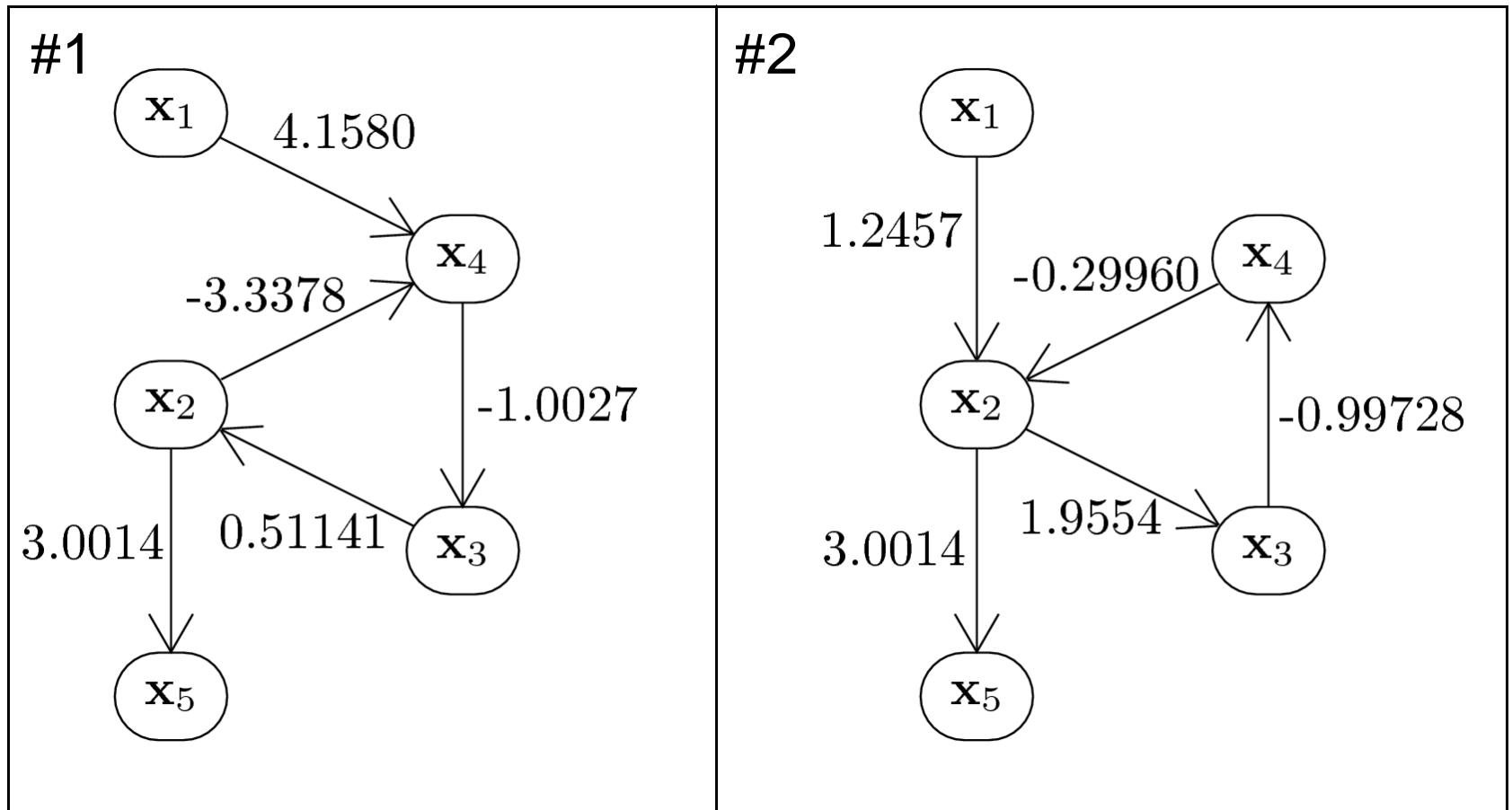
# LiNG-D: Demonstration

- Let's simulate using this model:
- Error terms are generated by sampling from a Gaussian and squaring
- 15000 data points
- We prune edges with coefficients  $< 0.05$
- Ready?



# LiNG-D: Demonstration

LiNG-D returns a set with 2 models:





# LiNG-D + the stability assumption

- Note that only one of these models is stable (assuming no self-loops).
- If our data is a set of equilibria, then the true model must be stable.
- How powerful is this constraint?

# LiNG-D + the stability assumption

- **Theorem:** if the true model's cycles don't intersect, then only one model is stable.
- For simple cycle models, cycle-products are inverted:  $c_1 = 1/c_2$ .
- So at least one cycle will be  $> 1$  (in modulus) and thus unstable.
- each cycle works independently, and any valid permutation\* will invert at least one cycle, creating an unstable model.

\*except for the identity permutation

# LiNG-D + the stability assumption

- Real data (*due to Zitian Wang*): 10-variable model, 28 edges
- LiNG-D tells us that 240 models explain the data equally well. That's too many!
- But only 2 are stable!
- Lesson: stability is a powerful constraint.
- Caveat: this assumes no-self loops (this is a strong assumption!)



# What should one use?

	non-Gaussian	Unknown <small>or both or too little data</small>	Gaussian				
DAG	<p>LINGAM</p> <p>unique model</p>	<p>Check out Hoyer et al (2008) (yesterday's poster session)</p>	<p>Constraint-based methods e.g. PC, CPC, SGS (or Geiger and Heckerman 1994 for a Bayesian alternative)</p> <p>d-separation equivalence class</p>				
DG	<p>LiNG-D 2 cases</p> <table border="1"> <tr> <td>acyclic</td> <td>unique model</td> </tr> <tr> <td>cyclic</td> <td>distribution-equivalence class</td> </tr> </table>	acyclic	unique model	cyclic	distribution-equivalence class	<p>?</p>	<p>Richardson's CCD</p> <p>very large class: not even covariance equivalent</p>
acyclic	unique model						
cyclic	distribution-equivalence class						



# Take-home message

- LiNGAM exploits non-Gaussianity in acyclic case to find a unique SEM (rather than d-sep equivalence class).
- Similarly, in the cyclic case, LiNG-D narrows the class to a distribution-equivalence class of SEMs.
- Still, there may be multiple SEMs.
- Stability can sometimes be used to rule out a good chunk of those.
- Thank you!

# Appendix 1: self-loops

- Equilibrium equations usually correspond with the dynamical equations.  
... BUT IF a self-loop has coefficient 1, we will get the wrong structure, and the predicted results of intervention will be wrong!
- self-loop coefficients are underdetermined.
- Our stability results only hold if we assume no self-loops.

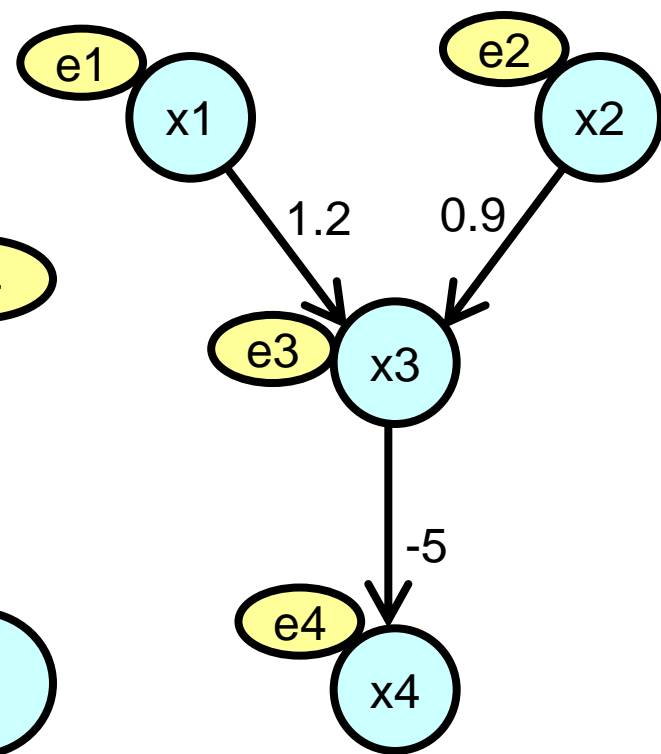
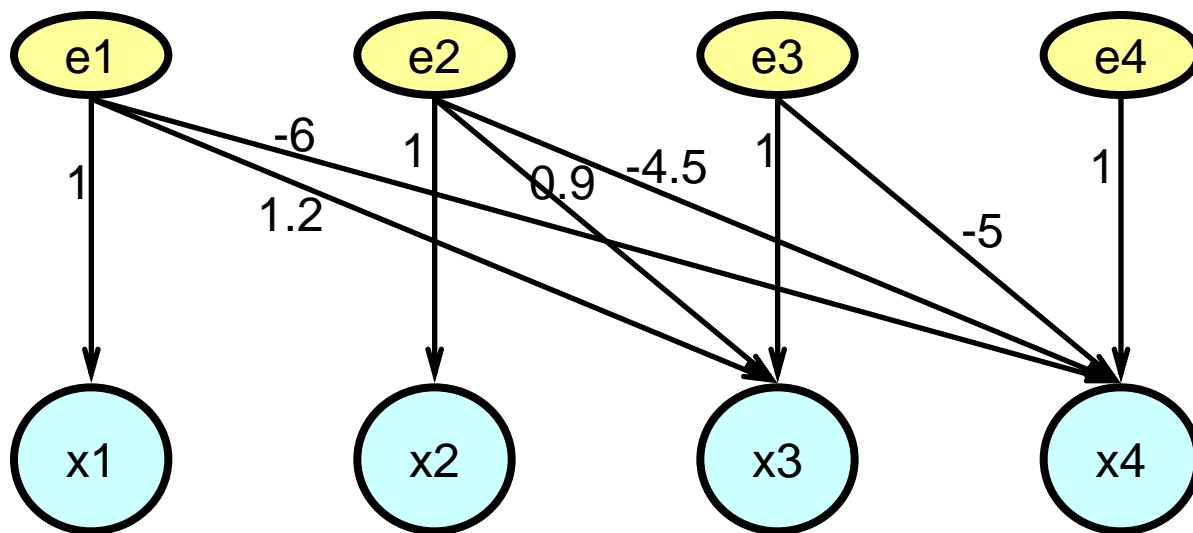
# Appendix 2: solving n-Rooks efficiently

- $W$  matrix: use hypothesis tests to turn all zeros to 0, all others to 1.
- Run a  $k$ -th best assignment algorithm, for increasing  $k$ , until you reach a suboptimal permutation (all good permutations will score exactly  $n$ )
- The time-complexity of this is the same as the  $k$ -best assignments problem.

# Linear Structural Equation Models (SEMs) (with randomness)

- The “mixing matrix” shows how the noise propagates:

Let's make it:



- Done.

# Why LiNGAM won't work

- Acyclic: there is a unique permutation of  $B$  with no zeros in the diagonal
- LiNGAM assigns a score
- Finds an ordering
  
- In cyclic case, we can't find an ordering, multiple permutations have a zeroless diagonal
  
- because:
  - since it assumes the data was generated by a DAG,
  - it searches for a single valid permutation