

# Directed Cyclic Graph for Causal Discovery from Multivariate Functional Data

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Statistics

Stat Café  
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## Joint work with



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# Why causality?

## Example 1

amazon prime Deliver to Snigdha Bryan 77801 All laptop bags

EN Hello, Saptanshi Account & Lists Returns & Orders 6 Cart

All Holiday Deals Medical Care Help Center Prime Video Amazon Basics Smart Home Household, Health & Baby Care Coupons All-new Echo Pop Kids: Now shipping

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Back to results



**Ferkurn 17 17.3 Inch Laptop Bag Women Men Computer Bag for HP Envy Pavilion Omen/LG Gram/MSI/Dell Inspiron XPS/Lenovo Thinkpad/ASUS/Acer, Shoulder Strap Carrying Briefcase Messenger Bag Large Case**

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# Why causality?

## Example 1

amazon prime Deliver to Snigdha Bryan 77801 All laptop bags

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All Holiday Deals Medical Care Help Center Prime Video Amazon Basics Smart Home Household, Health & Baby Care Coupons All-new Echo Pop Kids: Now shipping

Roll over image to zoom in

- Tips: 1--The product will have a little color difference in different screens. 2--There will be very small deviations due to the artificially measured size, please refer to the size of your laptop for purchase 3--If the laptop case is a bit spacious, the laptop shell may make it fit snugly.

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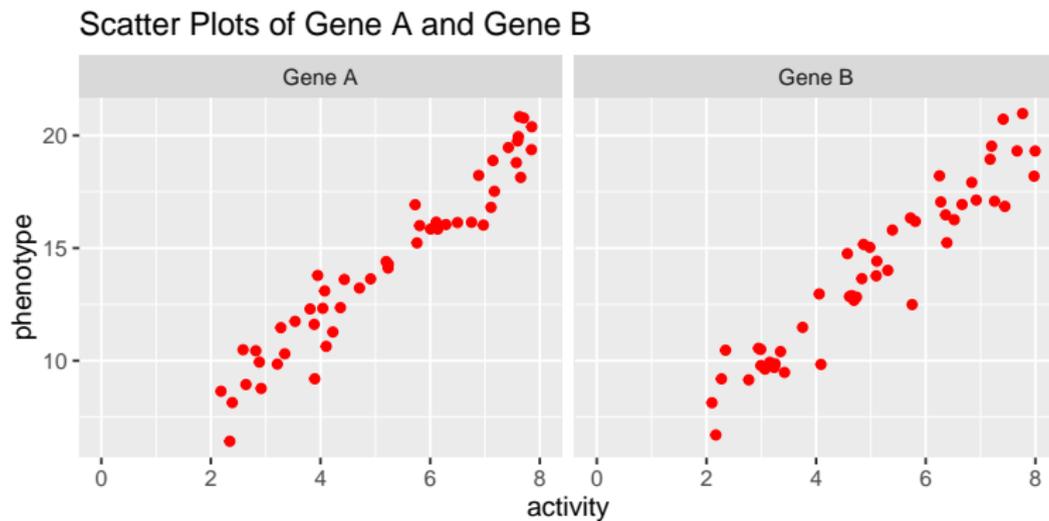
**This item:** Ferkurn 17 17.3 Inch Laptop Bag Women Men Computer Bag for HP Envy...  
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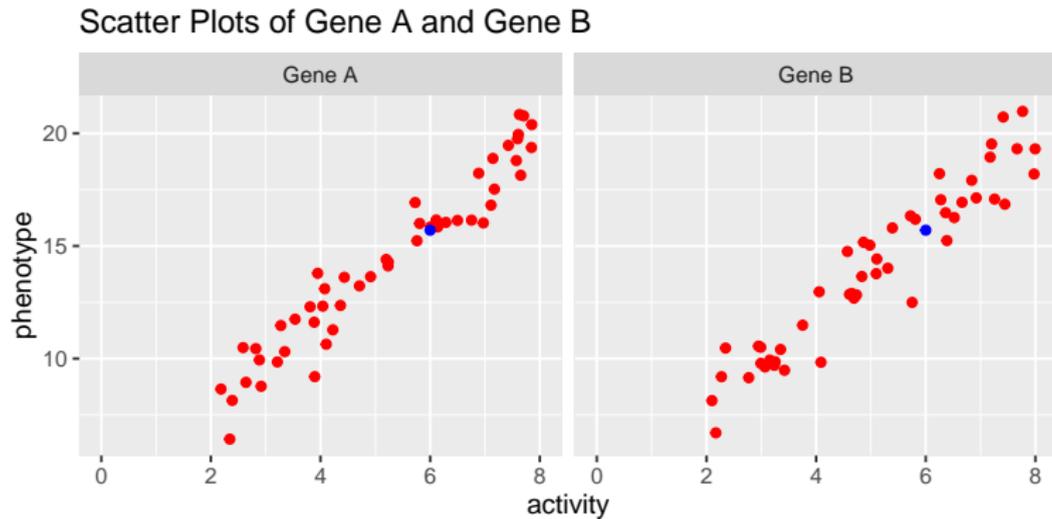
# Why causality?

## Example 2



# Why causality?

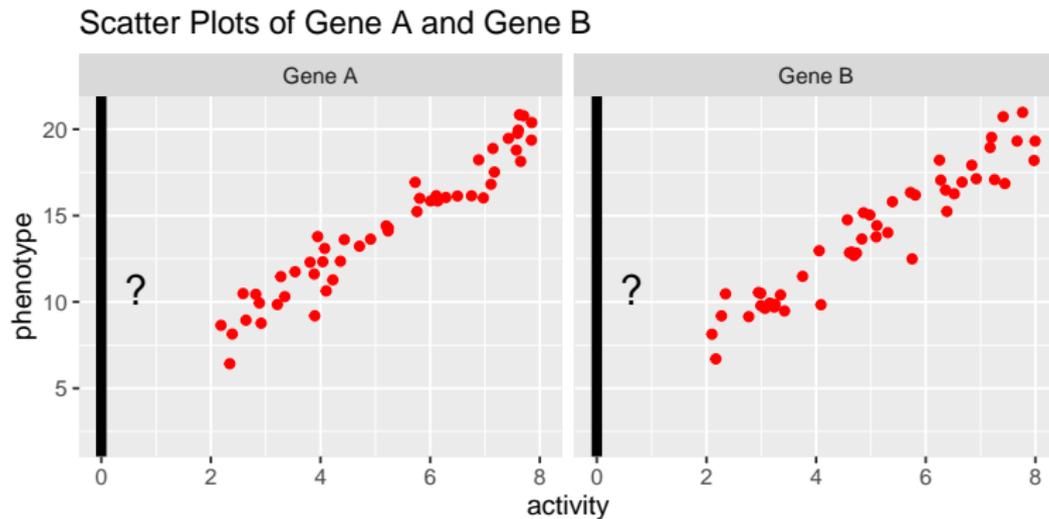
## Example 2



Statistical Question!!

# Why causality?

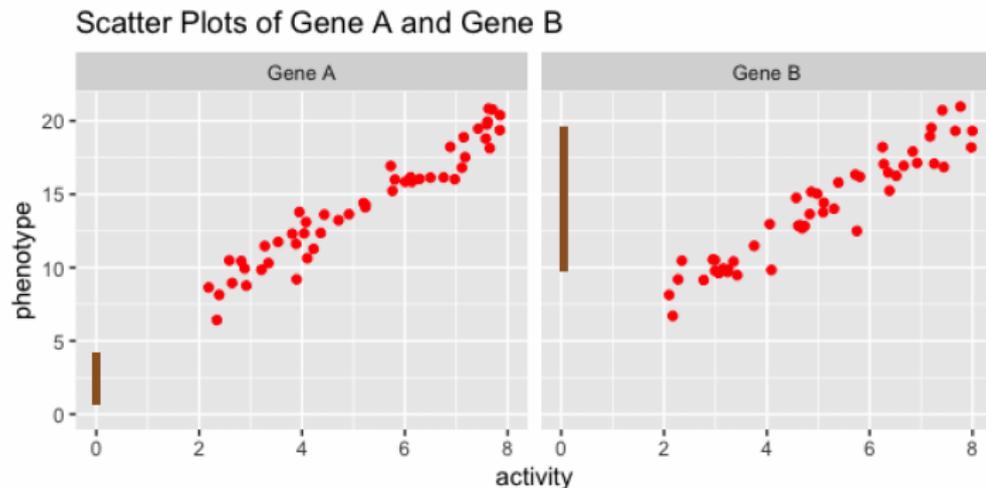
## Example 2



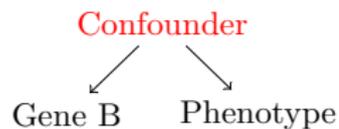
Causal Question!!

# Causality matters

## Example 2



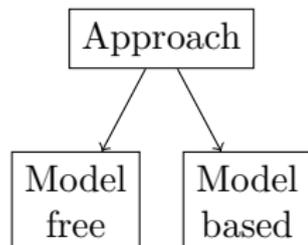
Gene A  $\longrightarrow$  Phenotype



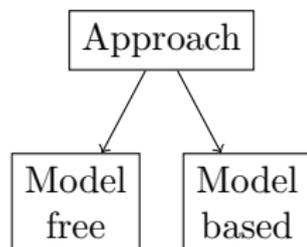
# Causal discovery

- ▶ Causal discovery - infer causal structure from data.
- ▶ Gold standard is experimental data, however mostly we have **observational data** at our disposal.
- ▶ Fairly a difficult task to do.
- ▶ Suppose  $X_1, \dots, X_p$  forms a graph  $\mathcal{G}$ . Goal is to learn  $\mathcal{G}$ .
- ▶ Some usual assumptions:-
  1. Causal Markov condition -  $X_i \perp\!\!\!\perp X_{\text{NonDesc}(i)} | X_{\text{pa}(i)}$ .  
smoking  $\rightarrow$  tissue damage  $\rightarrow$  lung cancer
  2. Causal faithfulness -  $X_i \perp\!\!\!\perp_p X_j | X_k \implies X_i \perp\!\!\!\perp_{\mathcal{G}} X_j | X_k$ .
  3. Causal sufficiency - Absence of any hidden confounders.
  4. Acyclicity - Use of Directed Acyclic Graphs (DAGs).

## Current approaches

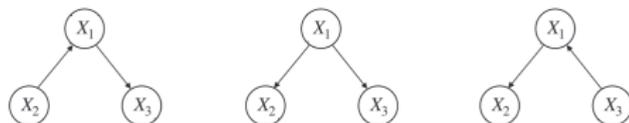


# Current approaches



## Model free approach:

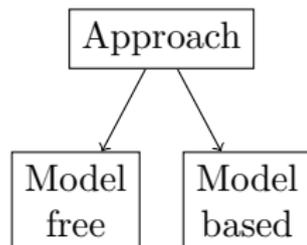
- ▶ Uses **conditional independence tests**
  - $\mathbf{X} \perp\!\!\!\perp \mathbf{Y} | \mathbf{Z}$ .
- ▶ Non-parametric approach.
- ▶ Assumptions: causal Markov condition, causal faithfulness.
- ▶ determines the orientations of the edges up to the **Markov equivalence class**.
- ▶ Examples: PC, FCI, CCD.



Markov equivalence class of trivariate graphs -  
 $X_2 \perp\!\!\!\perp X_3 | X_1$

**Question:** Can we do better than this?

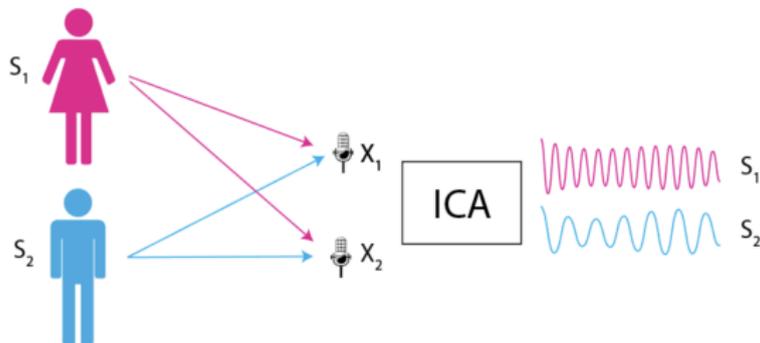
# Current approaches



## Model based approach:

- ▶ Structural equation model (SEM)  
 $X_i = f_i(\mathbf{X}_{\text{pa}(i)}, \epsilon_i)$ .
- ▶ Parametric approach.
- ▶ Restricts the function class.
- ▶ The causal model is fully identifiable.
- ▶ Examples - LiNGAM, LiNG, PNL, Non-linear Additive Noise models etc.
- ▶  $f(\mathbf{X}_{\text{pa}(i)}, \epsilon_i) = \mathbf{b}_i^\top \mathbf{X}_{\text{pa}(i)} + \epsilon_i$

# Independent component analysis



Goal is to recover the independent source signals  $S_i$ .

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

# ICA & LiNGAM

## ICA

- ▶ Model is  $\mathbf{X} = \mathbf{A}\mathbf{S}$ .
- ▶ Goal: to estimate  $\mathbf{W} = \mathbf{A}^{-1}$ .

## LiNGAM

- ▶ Model is  $(\mathbf{I} - \mathbf{B})\mathbf{X} = \mathbf{E}$ .
- ▶ Underlying graph structure is **acyclic**.
- ▶ Goal: to estimate  $\mathbf{B}$ .

# ICA & LiNGAM

## ICA

- ▶ Model is  $\mathbf{X} = \mathbf{AS}$ .
- ▶ Goal: to estimate  $\mathbf{W} = \mathbf{A}^{-1}$ .
- ▶  $S_i$  are non-gaussian and mutually independent.
- ▶ Identifiable upto **scaling** and **permutation** indeterminacy of indep. components  $\mathbf{S}$ .

$$\mathbf{X} = \underbrace{(\mathbf{APD})}_{\mathbf{A}^*} \underbrace{(\mathbf{D}^{-1}\mathbf{P}^\top \mathbf{S})}_{\mathbf{S}^*}$$

- ▶ several algorithms leads to efficient estimation of  $\mathbf{W}$ .

## LiNGAM

- ▶ Model is  $(\mathbf{I} - \mathbf{B})\mathbf{X} = \mathbf{E}$ .
- ▶ Underlying graph structure is **acyclic**.
- ▶ Goal: to estimate  $\mathbf{B}$ .

# ICA & LiNGAM

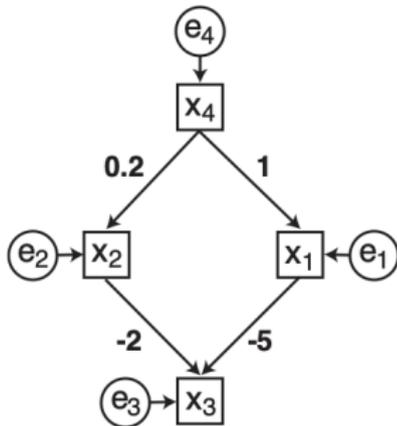
## ICA

- ▶ Model is  $\mathbf{X} = \mathbf{AS}$ .
- ▶ Goal: to estimate  $\mathbf{W} = \mathbf{A}^{-1}$ .
- ▶  $S_i$  are non-gaussian and mutually independent.
- ▶ Identifiable upto **scaling** and **permutation** indeterminacy of indep. components  $S$ .

$$\mathbf{X} = \underbrace{(\mathbf{APD})}_{\mathbf{A}^*} \underbrace{(\mathbf{D}^{-1}\mathbf{P}^\top \mathbf{S})}_{\mathbf{S}^*}$$

- ▶ several algorithms leads to efficient estimation of  $\mathbf{W}$ .

## LiNGAM



Unlike ICA, the **correct correspondence** between  $e_i$  and  $x_i$  is important in LiNGAM.

# ICA & LiNGAM

## ICA

- ▶ Model is  $\mathbf{X} = \mathbf{A}\mathbf{S}$ .
- ▶ Goal: to estimate  $\mathbf{W} = \mathbf{A}^{-1}$ .
- ▶  $S_i$  are non-gaussian and mutually independent.
- ▶ Identifiable upto **scaling** and **permutation** indeterminacy of indep. components  $\mathbf{S}$ .

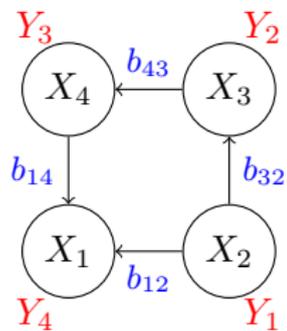
$$\mathbf{X} = \underbrace{(\mathbf{A}\mathbf{P}\mathbf{D})}_{\mathbf{A}^*} \underbrace{(\mathbf{D}^{-1}\mathbf{P}^\top \mathbf{S})}_{\mathbf{S}^*}$$

- ▶ several algorithms leads to efficient estimation of  $\mathbf{W}$ .

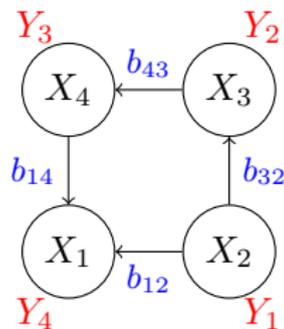
## LiNGAM

- ▶ Model is  $(\mathbf{I} - \mathbf{B})\mathbf{X} = \mathbf{E}$ .
- ▶ Underlying graph structure is **acyclic**.
- ▶ Goal: to estimate  $\mathbf{B}$ .
- ▶  $E_i$  are non-gaussian and mutually independent.
- ▶ Some post-processing needed on the  $\widehat{\mathbf{W}}$ .
- ▶ Efficient algorithm is provided in Shimizu et al. (2006).

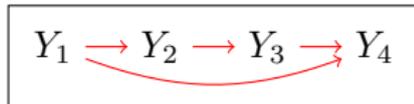
## Presence of cycles - Difficulty?



## Presence of cycles - Difficulty?

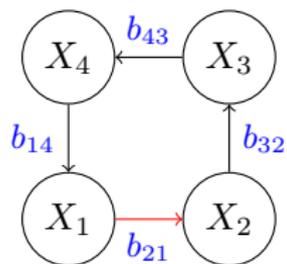
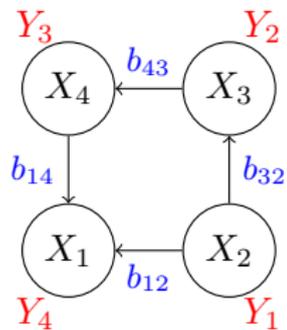


- ▶ DAGs iff topological order.
- ▶ Topological sort/order:  $Y_i \rightarrow Y_j \implies j > i$ .
- ▶ Example:  $Y_1(X_2) \ Y_2(X_3) \ Y_3(X_4) \ Y_4(X_1)$

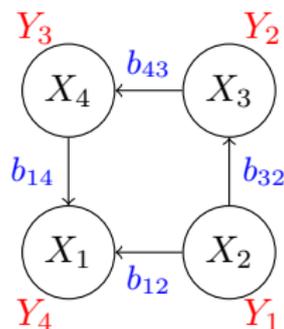


- ▶ 
$$\begin{pmatrix} Y_1 \\ \vdots \\ Y_4 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ b_{32} & 0 & 0 & 0 \\ 0 & b_{43} & 0 & 0 \\ b_{12} & 0 & b_{14} & 0 \end{pmatrix} \begin{pmatrix} Y_1 \\ \vdots \\ Y_4 \end{pmatrix} + \begin{pmatrix} e_2 \\ e_3 \\ e_4 \\ e_1 \end{pmatrix}$$
- ▶  $I - B$  is always invertible.

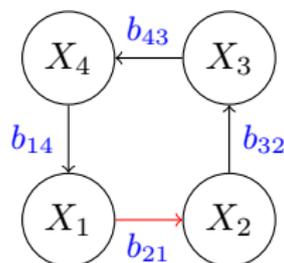
## Presence of cycles - Difficulty?



## Presence of cycles - Difficulty?



$$(\mathbf{I} - \mathbf{B})\mathbf{X} = \mathbf{E}$$



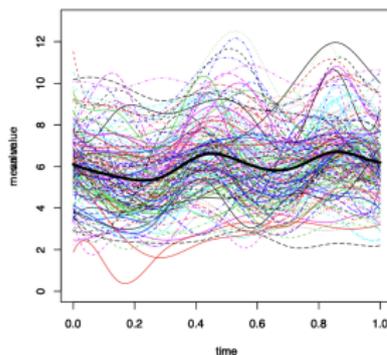
$$\mathbf{B} = \begin{pmatrix} 0 & 0 & 0 & b_{14} \\ b_{21} & 0 & 0 & 0 \\ 0 & b_{32} & 0 & 0 \\ 0 & 0 & b_{43} & 0 \end{pmatrix}$$

$$|\mathbf{I} - \mathbf{B}| = 1 - b_{14}b_{21}b_{32}b_{43}.$$

- ▶ Some extra conditions are necessary on  $\mathbf{B}$  to ensure invertibility.
- ▶ The moduli of the **eigenvalues** of  $\mathbf{B}$  are less than 1 and none equal to 1.

## Definition

- ▶ Data where the data points are itself functions or curves.
- ▶ A realization of a (typically smooth) random object that takes values in an abstract function space.
- ▶  $\mathcal{H} := \{X | X : \mathcal{T} \rightarrow [a, b]\}$ . Example: Hilbert space.
- ▶ Denoted by  $X = (X_1, \dots, X_p)^\top$ .
- ▶ Examples: 1) daily PM10 concentration curves recorded in Graz, Austria in winter season 2) electrical activity measured across different regions of the brain (EEG data).



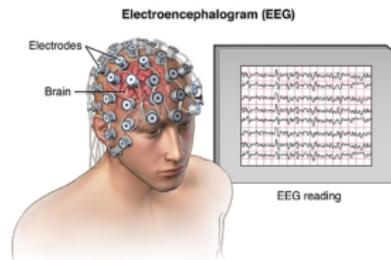
Source: Internet

# Challenges

1. Infinite-dimensionality of functional data
  - ▶ Low-freq spectrum of  $Y_j$  might causally affect the high-freq. spectrum of  $Y_\ell$ .
  - ▶ Demands identification of pertinent features.
  - ▶ The challenge is that we may not know *a priori* what these relevant features are.
2. Causal identifiability theory in presence of cycles/feedback loops.
3. Noisy functional data adds another layer of difficulty in probing the causal relationships of interest.

# Motivating example

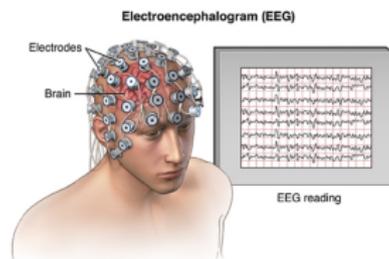
- ▶ Electroencephalography (EEG) data.



Source: Internet

# Motivating example

- ▶ Electroencephalography (EEG) data.
- ▶ Continuous and the short time separation between the adjacent measuring points.
- ▶ **Goal:** To estimate **brain effective connectivity** among different regions.
- ▶ Strong biological evidence behind presence of **feedback loops/cycles**.



Source: Internet

## Model definition

- ▶ Consider a multivariate stochastic process  $\mathbf{Y} = (Y_1, \dots, Y_p)^\top$  where each  $Y_j$  is defined on a compact domain  $\mathcal{T}_j \subset \mathbb{R}$ .
- ▶ Let  $Y_j \in \mathcal{H}_j$  where  $\mathcal{H}_j$  is a Hilbert space of functions defined on  $\mathcal{T}_j$ .
- ▶ Consider an operator-based non-recursive linear SEM on  $\mathbf{Y}$  as

$$Y_j(\cdot) = \sum_{\ell \in \text{pa}(j)} (\mathcal{B}_{j\ell} Y_\ell)(\cdot) + f_j(\cdot), \quad \forall j \in [p], \quad (1)$$

- ▶  $Y_\ell \rightarrow Y_j \implies \mathcal{B}_{j\ell} \neq 0$ . Assume  $\mathcal{B}_{jj}$  is a null operator (no self loops).
- ▶ Suppose if  $\mathbf{Y}_j \in \mathbb{R}^m \forall j$ , (1) is just,

$$\mathbf{Y}_j = \sum_{\ell \in \text{pa}(j)} \mathbf{B}_{j\ell} \mathbf{Y}_\ell + \mathbf{f}_j, \quad \forall j \in [p],$$

- ▶ However, model (1) is **infinite-dimensional** and hence challenging to estimate and interpret.

## Causal embedded space

- ▶ Assume that the causal relationships are preserved in an unknown low-dimensional subspace  $\mathcal{D}_j$  of  $\mathcal{H}_j$  of dim  $K_j$ .
- ▶  $\mathcal{P}_j$  and  $\mathcal{Q}_j$  are the projections onto  $\mathcal{D}_j$  and its orthogonal complement resp.
- ▶ Also assume  $\mathcal{B}_{j\ell} = \mathcal{P}_j \mathcal{B}_{j\ell} \mathcal{P}_\ell$ .
- ▶ As such, (1) can be split into

$$\begin{aligned}\mathcal{P}_j Y_j &= \sum_{\ell \in \text{pa}(j)} \mathcal{B}_{j\ell} (\mathcal{P}_\ell Y_\ell) + \mathcal{P}_j f_j, \\ \mathcal{Q}_j Y_j &= \mathcal{Q}_j f_j.\end{aligned}\tag{2}$$

- ▶ We assume that  $\mathcal{P}_j f_j$  and  $\mathcal{Q}_j f_j$  are independent of each other.

## Model definition

- ▶ In practice, we do not directly observe  $Y_j$ .
- ▶ For each  $Y_j$ , we observe  $\{(t_{ju}, X_{ju})\}_{u=1}^{m_j}$ , where  $X_{ju} \in \mathbb{R}$  is the measurement of  $Y_j$  at location  $t_{ju} \in \mathcal{T}_j$ .
- ▶ Therefore, we consider the following measurement model:

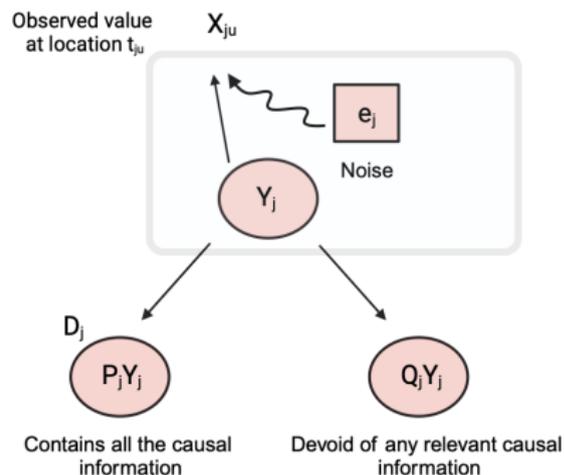
$$\begin{aligned} X_{ju} &= Y_j(t_{ju}) + e_{ju} \\ &= (\mathcal{P}_j Y_j)(t_{ju}) + (\mathcal{Q}_j Y_j)(t_{ju}) + e_{ju}, \quad \forall u \in [m_j], j \in [p], \end{aligned} \quad (3)$$

with independent noises  $e_{ju} \sim N(0, \sigma_j), \forall u \in [m_j]$ .

# Model definition

Recall that,

$$X_{ju} = (\mathcal{P}_j Y_j)(t_{ju}) + (\mathcal{Q}_j Y_j)(t_{ju}) + e_{ju}$$



# Model definition

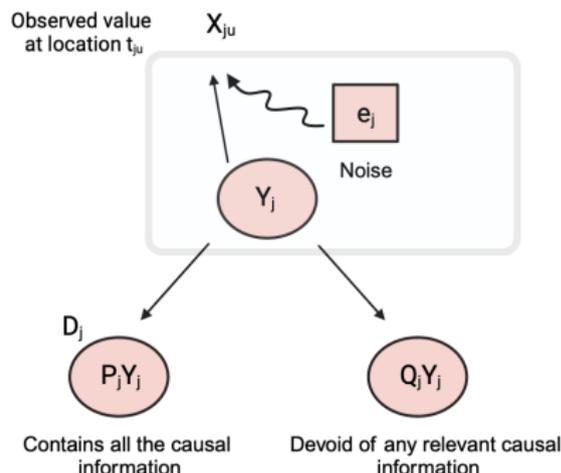
Recall that,

$$X_{ju} = (\mathcal{P}_j Y_j)(t_{ju}) + (\mathcal{Q}_j Y_j)(t_{ju}) + e_{ju}$$

- ▶ Define  $\alpha_j = \mathcal{P}_j Y_j$ ,  $\beta_j = \mathcal{Q}_j Y_j$  and  $\epsilon_j = \mathcal{P}_j f_j, \forall j \in [p]$ .
- ▶ More compactly,

$$\mathbf{X} = \boldsymbol{\alpha}(t) + \boldsymbol{\beta}(t) + \mathbf{e} \quad (4)$$

- ▶ **Question:** Is the proposed model **causally identifiable**?  
**Yes**, under certain assump.



# Assumptions

## Assumption 1 (Causal Sufficiency)

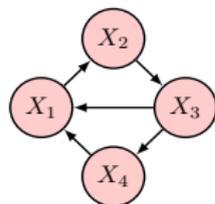
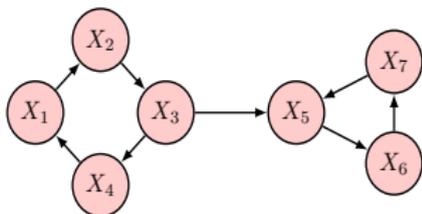
The model  $\mathcal{S} = (\mathcal{G}, \mathbb{P})$  is causally sufficient, i.e., there are no unmeasured confounders.

- ▶ Keeps the causal discovery task more manageable especially for cyclic graphs with purely observational data.

## Assumptions contd...

### Assumption 2 (Disjoint Cycles)

The cycles in  $\mathcal{G}$  are disjoint, i.e., no two cycles in the graph have two nodes that are common to both.



## Assumptions contd...

### Assumption 3 (Stability)

For the model  $\mathcal{S}$ , the moduli of the eigenvalues of the finite rank operator  $\mathcal{B}$  are less than or equal to 1, and none of the real eigenvalues are equal to 1.

- ▶ Similar kind of assumptions that were discussed for the univariate case have been extended for the random functions.

# Assumptions contd...

## Assumption 4 (Non-Gaussianity)

The exogenous variables have independent mixture of Gaussian distributions. i.e.,  $\epsilon_{jk} \stackrel{\text{ind}}{\sim} \sum_{m=1}^{M_{jk}} \pi_{jkm} \mathcal{N}(\mu_{jkm}, \tau_{jkm})$  with  $M_{jk} \geq 2$ .

- ▶ Can approx. any cont. distribution arbitrarily well <sup>1</sup>
- ▶ Useful as it induces model identifiability in the linear SEM framework.<sup>2</sup>

---

<sup>1</sup>Titterton, Smith, & Makov (1985). Statistical analysis of finite mixture distributions.

<sup>2</sup>Shimizu, Hoyer, Hyvärinen, & Kerminen. (2006). A Linear Non-Gaussian Acyclic Model for Causal Discovery.

## Assumptions contd...

Recall that,

$$X_{ju} = (\mathcal{P}_j Y_j)(t_{ju}) + (\mathcal{Q}_j Y_j)(t_{ju}) + e_{ju}$$

$$\beta_j = \mathcal{Q}_j Y_j$$

### Assumption 5 (Non-causal dependency)

Let  $\beta(\mathbf{t}) = \mathbf{C}(\mathbf{t})\gamma$ , where  $\mathbf{C}(\mathbf{t}) = \text{diag}(\mathbf{C}_{11}(\mathbf{t}_1), \dots, \mathbf{C}_{pp}(\mathbf{t}_p))$  and  $\gamma$  be another exogenous component. We assume

$$\gamma_{jk} \stackrel{\text{ind}}{\sim} \sum_{m=1}^{M_{jk}} \pi'_{jkm} \mathbf{N}(\mu'_{jkm}, \tau'_{jkm}) \text{ with } M_{jk} \geq 1.$$

- ▶  $\beta_j(\mathbf{t}_j) \perp\!\!\!\perp \beta_\ell(\mathbf{t}_\ell)$  for  $j \neq \ell$  and  $j, \ell \in [p]$ .
- ▶  $\mathbf{C}_{jj}(\mathbf{t}_j)$  mixes the independent entries in  $\gamma$  to generate temporal dependence within  $\beta_j(\mathbf{t}_j)$ .

## Assumptions contd...

Recall,  $\mathbf{X} = \boldsymbol{\alpha}(\mathbf{t}) + \boldsymbol{\beta}(\mathbf{t}) + \mathbf{e}$ . Then if  $\alpha_j(t_{ju}) = \sum_{k=1}^{K_j} \tilde{\alpha}_{jk} \phi_{jk}(t_{ju})$ , then (4) can be written as,

$$\mathbf{X} = \boldsymbol{\Phi}(\mathbf{t})\tilde{\boldsymbol{\alpha}} + \boldsymbol{\beta}(\mathbf{t}) + \mathbf{e},$$

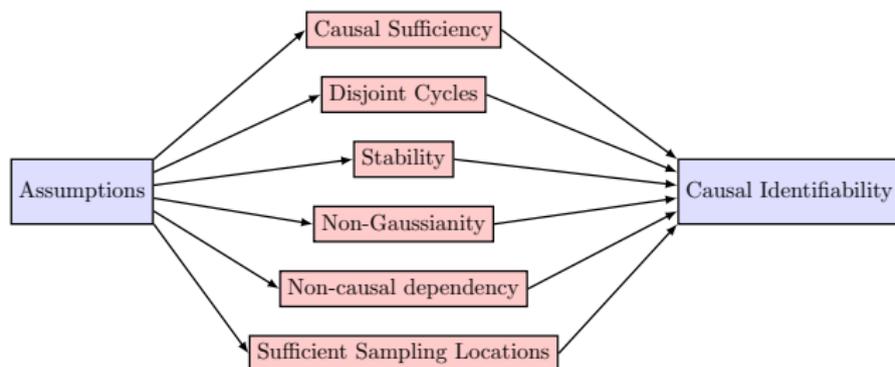
where  $\boldsymbol{\Phi}(\mathbf{t}) = \text{diag}(\boldsymbol{\Phi}_1(\mathbf{t}_1), \dots, \boldsymbol{\Phi}_p(\mathbf{t}_p))$  with  $\boldsymbol{\Phi}_j(\mathbf{t}_j) = (\phi_{jv}(t_{ju}))_{u,v=1}^{m_j, K_j}$ .

### Assumption 6 (Sufficient sampling locations)

The basis matrix  $\boldsymbol{\Phi}(\mathbf{t})$  of size  $\sum_{j=1}^p m_j \times \sum_{j=1}^p K_j$  has a full column rank.

- ▶ Implies enough sampling locations over which each random function  $Y_j$  is observed.
- ▶ Captures all the pertinent causal information that  $Y_j$  contains.

# Main theorem



## Theorem (Causal Identifiability)

Under Assumptions 1-6,  $\mathcal{S} = (\mathcal{G}, \mathbb{P})$  is causally identifiable.

## Inference - Model parameters

- ▶  $\mathbf{E} = (E_{j\ell})_{j,\ell=1}^p$  denote the adjacency matrix.
- ▶  $X_{ju} = Y_j(t_{ju}) + e_{ju}$ ,  $e_{ju} \sim \mathcal{N}(0, \sigma_j)$
- ▶ Suppose  $Y_j = \sum_{k=1}^S \tilde{\alpha}_{jk} \phi_k$ .
- ▶ We define SEM on first  $K_j$  components.

$$\tilde{\boldsymbol{\alpha}} = \mathbf{B} \tilde{\boldsymbol{\alpha}} + \tilde{\boldsymbol{\epsilon}}$$

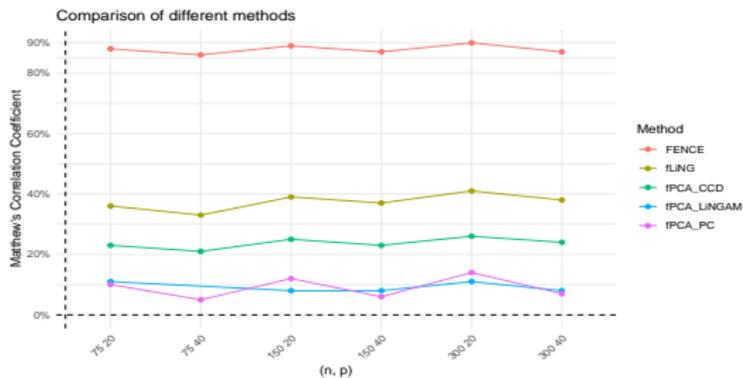
where  $\tilde{\boldsymbol{\alpha}}_j = (\tilde{\alpha}_{j1}, \dots, \tilde{\alpha}_{jK_j})^\top$  and  $\tilde{\boldsymbol{\alpha}} = (\tilde{\boldsymbol{\alpha}}_1, \dots, \tilde{\boldsymbol{\alpha}}_p$ .

- ▶  $\phi_k$ 's are useful for restricting each  $Y_j$  to  $D_j$ . Do **not** fix them.
- ▶ Further expand them with known cubic b-spline basis functions,  $\phi_k(\cdot) = \sum_{r=1}^R A_{kr} b_r(\cdot)$ .
- ▶  $\epsilon_{jk} \stackrel{\text{ind}}{\sim} \sum_{m=1}^{M_{jk}} \pi_{jkm} \mathcal{N}(\mu_{jkm}, \tau_{jkm})$ .
- ▶ Some very std. priors are taken to formulate the Bayesian procedure.

## Simulation study setup

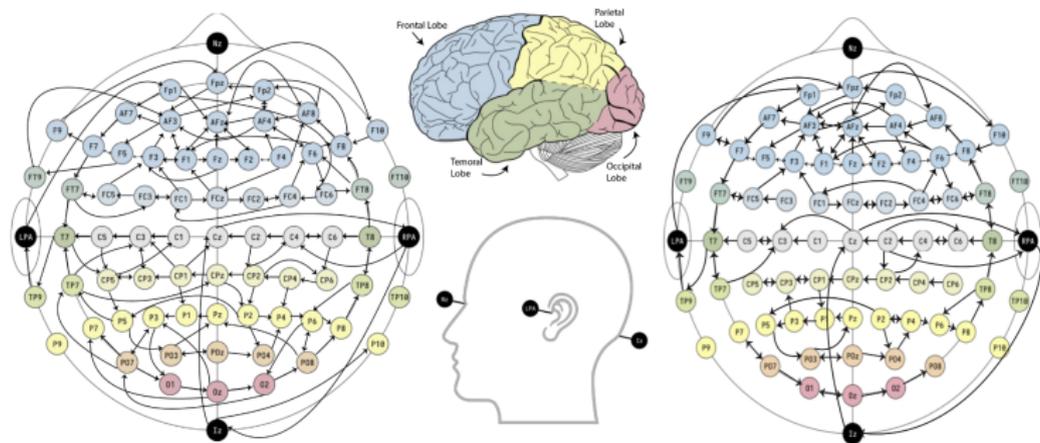
- ▶ Sample size ( $n$ ) = {75, 150, 300}, number of nodes ( $p$ ) = {20, 40}, time grid size ( $d$ ) = 125.
- ▶ The causal graph  $G$  is estimated by thresholding the posterior probability of inclusion at 0.5.
- ▶ Methods compared against:
  1. Functional Bayesian Network (fLiNG).
  2. fPCA-CCD
  3. fPCA-PC
  4. fPCA-LiNGAM
- ▶ 2, 3 and 4 are two step procedures:
  - **First step** involves obtaining the basis coefficients by carrying out fPCA.
  - **Second step** involves estimating the causal graphs using existing causal discovery methods.

# Results



- ▶ We used Matthew's correlation coefficient (MCC) to assess the graph recovery performance.

# Application - EEG Data



- ▶ For both groups (alcoholic and control), brain regions that are **spatially closer** to each other tend to be more connected.
- ▶ Dense connectivity is observed in the **frontal region** of the brain in both groups, with multiple cycles being formed.
- ▶ Alcoholic group has more connectivity across the left parietal and occipital lobes.

# Conclusions

- ▶ Proposed an operator-based non-recursive linear SEM based framework for functional data in the presence of cycles.
- ▶ Introduced the assumption of existence of a lower dimensional causal embedded space that captures all the causal information.
- ▶ Proved causal identifiability of our model under certain assumptions.
- ▶ Showed applications over an EEG dataset.

## **Future directions:**

- ▶ Relaxing the assumption for causal sufficiency.
- ▶ Consider non linear SEM framework.

## Reference

Roy, S., Wong, R. K. W., & Ni, Y. (2023). Directed Cyclic Graph for Causal Discovery from Multivariate Functional Data. Accepted in NeurIPS, 2023.



Thank you!

**Backup slides**

## Why stability assumption?

- ▶ We assume our data are drawn from an equilibrium distribution of a dynamic system involving multivariate functions.
- ▶  $\mathbf{Y}(\cdot)[t] = (Y_1(\cdot)[t], \dots, Y_p(\cdot)[t])^\top$  denote a vector of functions at time point  $t$  where the domain of each function  $Y_j(\cdot)[t]$  is not necessarily time.
- ▶ we have used  $(\cdot)$  to denote the function input/domain and  $[]$  to denote the time index of a dynamic system.
- ▶ Consider an AR1-type dynamic system of those functions,

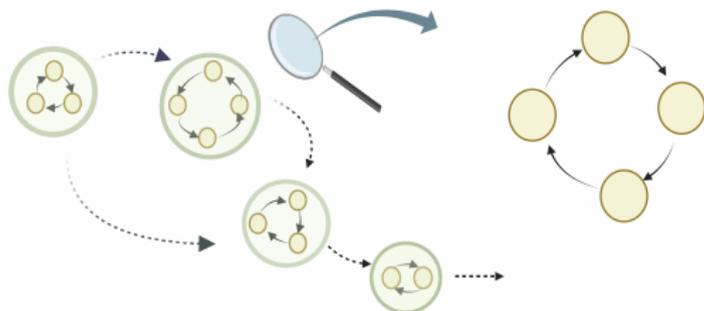
$$\mathbf{Y}(\cdot)[t] = \mathfrak{B}\mathbf{Y}(\cdot)[t-1] + \mathbf{f}(\cdot)$$

- ▶ Recursively leads to,

$$\mathbf{Y}(\cdot)[t] = \mathfrak{B}^t \mathbf{Y}(\cdot)[0] + \sum_{s=0}^{t-1} \mathfrak{B}^s \mathbf{f}(\cdot)$$

- ▶  $\mathfrak{B}^t$  and  $\sum_{s=0}^{t-1} \mathfrak{B}^s$  converge as  $t$  approaches infinity.

## Proof – A brief sketch pictorially



- ▶ In LHS, a **hypergraph**-like structure emerges when we assume the existence of **disjoint cycles**.
- ▶ While the true graph contains cycles, this hypergraph-like structure is essentially a **DAG**, thus easier to work with.
- ▶ LHS to RHS.

# Prior specifications

## Prior on spline coefficients $\mathbf{A}_k$

$$\mathbf{A}_k | \lambda_k \sim \mathbf{N}(\mathbf{0}, \lambda_k^{-1} \mathbf{\Omega}^-)$$

where  $\mathbf{\Omega}^-$  is the pseudoinverse of  $\mathbf{\Omega} = \int \mathbf{b}''(t) [\mathbf{b}''(t)]^\top dt$ . We constrain the regularization parameters  $\lambda_1 > \dots > \lambda_S > 0$  by putting a uniform prior:

$$\begin{aligned} \lambda_k &\sim \text{Uniform}(L_k, U_k), \quad \forall k \in [S], \\ U_1 &= 10^8, L_k = \lambda_{k+1} \quad \forall k \in [S-1], \\ U_k &= \lambda_{k-1} \quad \forall k \in \{2, \dots, S\}, L_S = 10^{-8}, \end{aligned}$$

which implies that the smoothness of  $\phi_k(\cdot)$  decreases as  $k$  gets larger.

# Prior specifications

## Prior on adjacency matrix $\mathbf{E}$

$$E_{j\ell} | \rho \stackrel{\text{ind}}{\sim} \text{Bernoulli}(\rho)$$
$$\rho \sim \text{Uniform}(0, 1)$$

- ▶ The marginal distribution of  $\mathbf{E}$  with  $\rho$  integrated out is  $\text{Beta} \left( \sum_{j \neq \ell} E_{j\ell} + 1, \sum_{j \neq \ell} (1 - E_{j\ell}) + 1 \right)$ .
- ▶ If  $\mathbf{E}_0$  denotes the null adj. matrix and  $\mathbf{E}_1$  denotes the adj. matrix with only one edge, then we can see that  $p(\mathbf{E}_0)/p(\mathbf{E}_1) = p^2 - p$ .
- ▶ prevents false discoveries and leads to a sparse network by increasing the penalty against additional edges as the dimension  $p$  grows.

# Prior specifications

## Prior on the causal effect matrix $\mathbf{B}$

$$\mathbf{B}_{j\ell} | E_{j\ell} \sim (1 - E_{j\ell})MVN(\mathbf{B}_{j\ell}; \mathbf{0}, s\gamma \mathbf{I}_{K_j}, \mathbf{I}_{K_\ell}) + E_{j\ell}MVN(\mathbf{B}_{j\ell}; \mathbf{0}, \gamma \mathbf{I}_{K_j}, \mathbf{I}_{K_\ell})$$
$$\gamma \sim \text{IG}(a_\gamma, b_\gamma)$$

with  $s = 0.02, a_\gamma = b_\gamma = 1$ .

- ▶ continuous spike and slab prior.
- ▶ When  $E_{j\ell} = 0$ ,  $\mathbf{B}_{j\ell}$  is negligibly small.

## Prior on the noise variances $\sigma_j$

$$\sigma_j \sim \text{IG}(a_\sigma, b_\sigma)$$

with  $a_\sigma = b_\sigma = 0.01$ .

# Prior specifications

## Prior on the mixture distribution parameters

$$(\pi_{jk1}, \dots, \pi_{jkM_{jk}}) \sim \text{Dirichlet}(\beta, \dots, \beta), \quad \forall j \in [p], k \in [S]$$

$$\mu_{jkm} \sim N(a_\mu, b_\mu), \quad \tau_{jkm} \sim \text{IG}(a_\tau, b_\tau), \quad \forall j \in [p], k \in [S], m \in [M_{jk}]$$

We have fixed values for the hyperparameters,  $\beta = 1$ ,  
 $a_\mu = 0, b_\mu = 100, a_\tau = b_\tau = 1$ .

## Choice of $K_j$

- ▶ Possible to use a prior to learn the number of basis functions jointly with other parameters.
- ▶ The functional observations are imputed and arranged into a  $(n \times p) \times d$  matrix, where  $d = |\cup_{i,j} \mathcal{T}_j^{(i)}|$  represents the size of the union of the measurement grid over all realized random functions.
- ▶ Singular value decomposition is performed, and the minimum value of  $K$  is selected such that its proportion of variance explained is at least 90%.
- ▶ We set  $K_j = K$ . Note that although  $K$  is fixed, the basis functions are adaptively inferred.
- ▶ Fix a grid encompassing values  $\{1, 2, 3, 4, 5, 6, 7\}$  for  $K$  and subsequently selecting the  $K$  associated with the lowest WAIC.
- ▶ The graph recovery performance remains almost the same.