## Discoverability with Modern Al

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## Problem Statement

How can we enhance discoverability with modern causal AI?

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**Discoverability** is the ability to find previously unknown **reliable** causal relationships, or lack thereof, in correlational data.

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**Discoverability** is the ability to find previously unknown **reliable** causal relationships, or lack thereof, in correlational data.

**Reliability** can be measured by the statistical likelihood that a suggested relationship holds true.

# Agenda

- Motivation
- 2 Background
- Project Overview
- 4 Impact of Assumption Violations
- 5 Detecting Assumption Violations
- 6 Examples
- Future Work
  - Interface

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## Motivation

#### Patterns can be misleading:

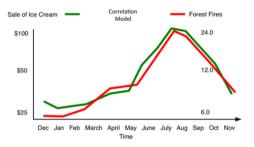


Figure 1: Ice cream causes forest fires?[1]

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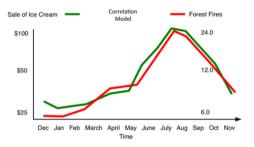


Figure 1: Ice cream causes forest fires?[1]

#### Critical areas:

- Healthcare
- Education
- Environmental science
- Crime

#### Patterns can be misleading:



Figure 1: Ice cream causes forest fires?[1]

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- Healthcare
- Education
- Environmental science
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#### **Experiments can be:**

- Costly
- Impractical
- Unethical

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DirectLiNGAM

## DirectLiNGAM Overview

#### Causal inference algorithm [2]

	×0	×1	x2	x3
0	1.5	3.4	1.3	0.1
1	2.6	3.5	1.6	0.8
2	1.2	3.4	1.3	0.6
3	1.7	3.5	1.5	0.7
4	1.2	3.4	1.3	0.1
5	1.7	3.5	1.5	0.8
6	1.5	3.4	1.3	0.9

Table 1: Multivariate data

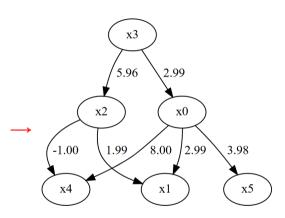


Figure 2: Causal graph

Linearity

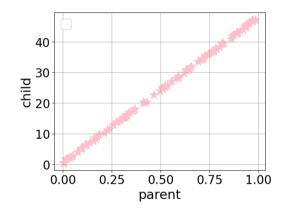


Figure 3: **child** = **a** \* **parent** + **noise** 

- Linearity
- Non-Gaussianity

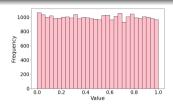


Figure 3: Non-Gaussian distribution

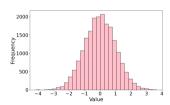


Figure 4: Gaussian distribution

- Linearity
- Non-Gaussianity
- Acyclicity

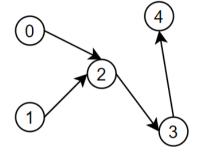


Figure 3: A directed acyclic graph

- Linearity
- Non-Gaussianity
- Acyclicity
- No hidden confounders

#### True Relationship Observed Relationship

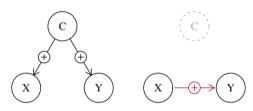


Figure 3: Confounders in causal relationships

- Linearity
- Non-Gaussianity
- Acyclicity
- No hidden confounders
- Infinite data

"[DirectLiNGAM] is guaranteed to converge to the right solution within a small fixed number of steps if the data strictly follows [these assumptions]." [2]

## DirectLiNGAM Breakdown

- Create hierarchy
- Find variable relationships [3]

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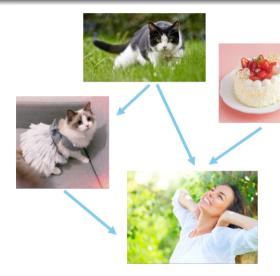
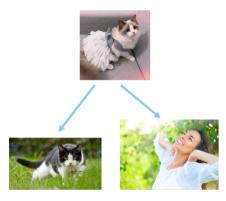


Figure 3: Example relationships

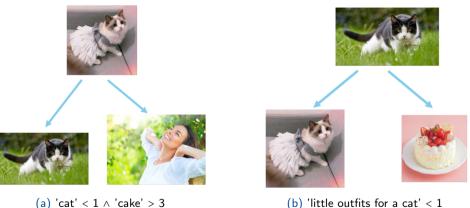
Fujitsu Causal Discovery = DirectLiNGAM + Conditions

#### Fujitsu Causal Discovery = DirectLiNGAM + Conditions



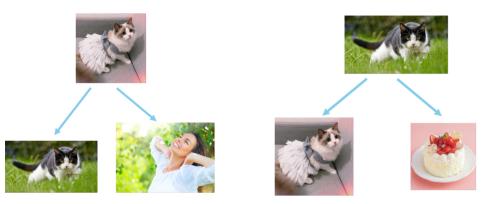
(a) 'cat'  $< 1 \land$  'cake' > 3

#### Fujitsu Causal Discovery = DirectLiNGAM + Conditions



(b) 'little outfits for a cat' < 1

### Fujitsu Causal Discovery = DirectLiNGAM + Conditions



(a) 'cat'  $< 1 \land$  'cake' > 3

(b) 'little outfits for a cat' < 1

### ⇒ Fill gaps left by DirectLiNGAM

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**Q:** How do we quantify reliability?

# **Project Components**

• Impact of assumption violations

## **Project Components**

• Impact of assumption violations

Detect violations

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- Impact of assumption violations
- Detect violations
- Create scoring metric

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#### Configurable properties:

- Dataset size
- Linear/nonlinear relationships
- Gaussian/non-Gaussian noise
- Confounders
- Cycles

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- Dataset size
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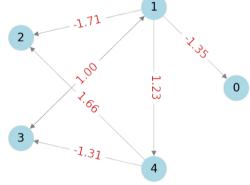


Figure 5: A causal graph with five nodes, generated using causally

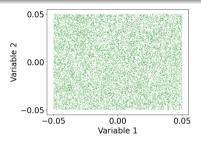


Figure 6: Dataset1280

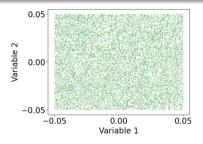


Figure 6: Dataset1280

dataset_name	num_rows	num_cols	noise_type	linearity	confounders	cycles
dataset1279	20000	2	uniform	nonlinear	1	0
dataset1280	20000	2	uniform	nonlinear	1	1
dataset1281	30	3	normal	linear	0	0
dataset1282	30	3	normal	linear	0	1

Table 2: Dataset metadata

### Accuracy Metric

#### Record accuracy[4]





(b) DirectLiNGAM

$$F1 = \frac{TP}{TP + 0.5(FP + FN)} = \frac{3}{4}$$

#### Find Accuracy For All Datasets

#### Use Fujitsu Causal Discovery on generated data

dataset_name	noise_type	linearity	cycles	F1
dataset790	normal	nonlinear	1	0.667
dataset2629	normal	linear	0	0.800
dataset2687	normal	nonlinear	0	0.667
dataset2761	uniform	linear	0	0.909
dataset2946	normal	linear	1	0.750
dataset256	uniform	nonlinear	1	0.000
dataset3754	uniform	linear	1	0.600
dataset3815	uniform	nonlinear	0	1.000

Table 3: Performance (F1 score) of different datasets.

## Sensitivity Analysis- Linear Model



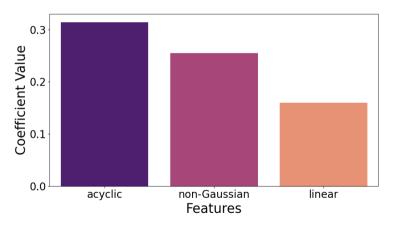


Figure 8: Coefficients for the linear model predicting F1 score

# Sensitivity Analysis

Develop a scoring metric:

 $\begin{cases} 0: \text{violates assumption} \\ 1: \text{does not violate assumption} \end{cases}$ 

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Develop a scoring metric:

$$\begin{cases} 0: \text{violates assumption} \\ 1: \text{does not violate assumption} \end{cases}$$
 
$$R = .3141(\text{acyclic}) + .2552(\text{non-Gaussian}) + .1602(\text{linear}) \tag{1}$$

#### Sensitivity Analysis

#### Develop a scoring metric:

$$\begin{cases} 0: \text{violates assumption} \\ 1: \text{does not violate assumption} \end{cases}$$
 
$$R = .3141(\text{acyclic}) + .2552(\text{non-Gaussian}) + .1602(\text{linear})$$
 (1)

Reliability = 
$$\frac{R}{.7295}$$
 = Estimated F1

## Sensitivity Analysis - Example Dataset



Figure 9: Cats-DirectLiNGAM violations

 $\implies \begin{cases} \mathsf{acyclic: 0} \\ \mathsf{non\text{-}Gaussian: 1} \\ \mathsf{linear: 0} \end{cases}$ 

## Sensitivity Analysis - Example Dataset

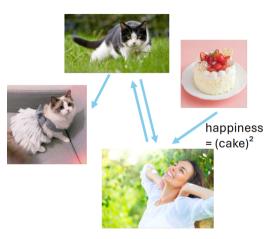


Figure 9: Cats-DirectLiNGAM violations

$$\Longrightarrow \begin{cases} \mathsf{acyclic:} \ 0 \\ \mathsf{non-Gaussian:} \ 1 \\ \mathsf{linear:} \ 0 \end{cases}$$

$$R = .3141(acyclic) + .2552(non-Gaussian)$$
  
  $+ .1602(linear)$   
  $= .3141(0) + .2552(1) + .1602(0)$   
  $= .2552$ ,

### Sensitivity Analysis - Example Dataset



Figure 9: Cats-DirectLiNGAM violations

$$\Longrightarrow \begin{cases} \mathsf{acyclic:} \ 0 \\ \mathsf{non\text{-}Gaussian:} \ 1 \\ \mathsf{linear:} \ 0 \end{cases}$$

$$R = .3141(acyclic) + .2552(non-Gaussian)$$
  
+  $.1602(linear)$   
=  $.3141(0) + .2552(1) + .1602(0)$   
=  $.2552$ ,

→ **reliability** = 
$$\frac{.2552}{.7295}$$
 = .3498

## **Grading Scale**

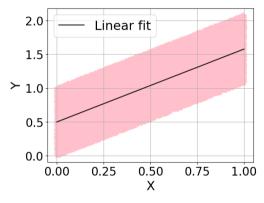
acyclic	non-Gaussian	linear	reliability	grade
0	0	0	0.0000	F
0	0	1	0.2196	F
0	1	0	0.3498	F
0	1	1	0.5694	D
1	0	0	0.4306	F
1	0	1	0.6502	C
1	1	0	0.7804	В
1	1	1	1.0000	Α

Table 4: Possible reliability scores and associated grades

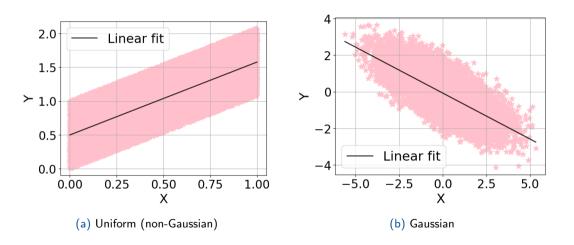
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(a) Uniform (non-Gaussian)



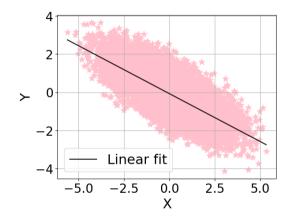


Figure 11: Gaussian

Success rate: 74.7%

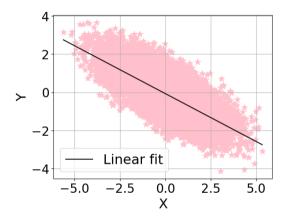


Figure 11: Gaussian

Success rate: 74.7%

 For each pair of variables, calculate a line of best fit and record the residuals

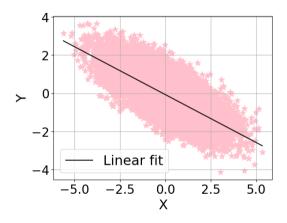


Figure 11: Gaussian

Success rate: 74.7%

- For each pair of variables, calculate a line of best fit and record the residuals
- Perform a Shapiro-Wilk test on these values [5]

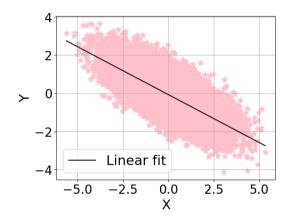


Figure 11: Gaussian

Success rate: 74.7%

- For each pair of variables, calculate a line of best fit and record the residuals
- Perform a Shapiro-Wilk test on these values [5]
- If any pair presents Gaussian noise: dataset → Gaussian

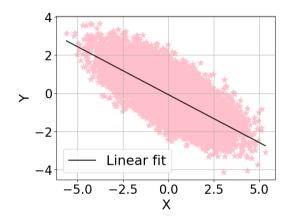


Figure 11: Gaussian

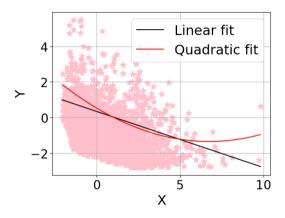


Figure 12: non-linearity

Success rate: 68.4%

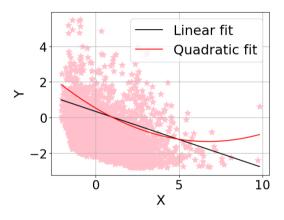


Figure 12: non-linearity

Success rate: 68.4%

Fit a polynomial, of increasing degrees, to each pair of variables using an orthogonal basis [6].

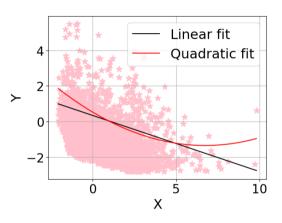


Figure 12: non-linearity

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Fit a polynomial, of increasing degrees, to each pair of variables using an orthogonal basis [6].

A pair is defined as:

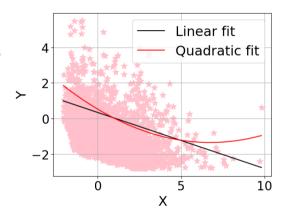


Figure 12: non-linearity

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A pair is defined as:

• Nonlinear: degree 2-9

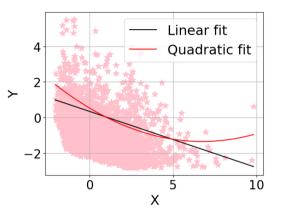


Figure 12: non-linearity

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Fit a polynomial, of increasing degrees, to each pair of variables using an orthogonal basis [6].

A pair is defined as:

• Nonlinear: degree 2-9

• Linear: degree 1

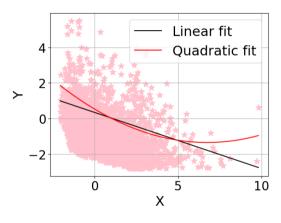


Figure 12: non-linearity

Success rate: 68.4%

Fit a polynomial, of increasing degrees, to each pair of variables using an orthogonal basis [6].

A pair is defined as:

Nonlinear: degree 2-9

• Linear: degree 1

• Unrelated: degree 9

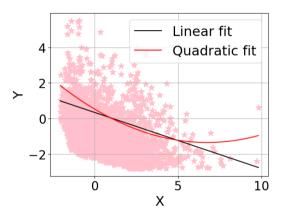


Figure 12: non-linearity

Success rate: 48.6%

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If a pair of variables:

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If a pair of variables:

- has a high correlation coefficient,
- has no link found by DirectLiNGAM,
- is not caused by other variables,

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then the dataset is confounded.

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If a pair of variables:

- has a high correlation coefficient,
- has no link found by DirectLiNGAM,
- is not caused by other variables,

then the dataset is confounded.

	Not confounded	Confounded
Predicted not confounded	1712	1799
Predicted confounded	208	121

Table 5: Results of confoundedness test on generated data

Success rate:  $36.4\% \rightarrow 63.6\%$ 

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To detect cycles:

23

Success rate:  $36.4\% \rightarrow 63.6\%$ 

To detect cycles:

Run DirectLiNGAM

23

Success rate:  $36.4\% \rightarrow 63.6\%$ 

#### To detect cycles:

Run DirectLiNGAM

Repeat, with prior knowledge, once for each variable

Success rate:  $36.4\% \rightarrow 63.6\%$ 

#### To detect cycles:

- Run DirectLiNGAM
- 2 Repeat, with prior knowledge, once for each variable
- For each potential relationship find:
  - # of times allowed
  - ullet # of times predicted

Success rate:  $36.4\% \rightarrow 63.6\%$ 

#### To detect cycles:

- Run DirectLiNGAM
- 2 Repeat, with prior knowledge, once for each variable
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  - # of times allowed
  - # of times predicted
- Compare ratio to threshold

### Detecting Assumption Violations - Cycles Test

Success rate:  $36.4\% \rightarrow 63.6\%$ 

#### To detect cycles:

- Run DirectLiNGAM
- 2 Repeat, with prior knowledge, once for each variable
- For each potential relationship find:
  - # of times allowed
  - # of times predicted
- Compare ratio to threshold

	Acyclic	Cyclic
Predicted acyclic	38	561
Predicted cyclic	1882	1359

Table 6: Results of cyclicity test on generated data

Success rate: 100%

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Check for the proportion of columns to rows.

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$$P = \frac{\text{number of columns}}{\text{number of rows}},$$

Success rate: 100%

Check for the proportion of columns to rows.

$$P = \frac{\text{number of columns}}{\text{number of rows}},$$

which means a smaller number fits the assumption better.

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# Using our tool on real data!

Altitude vs. Temperature

Grade:  $43\% \rightarrow \mathbf{F}$ 

Horsepower vs. MPG

Grade:  $78\% \rightarrow \mathbf{B}$ 

Altitude vs. Temperature Grade:  $43\% \rightarrow \mathbf{F}$ 

What contributed to these scores?

Horsepower vs. MPG Grade:  $78\% \rightarrow \mathbf{B}$ 

Altitude vs. Temperature Grade:  $43\% \rightarrow \mathbf{F}$ 

What contributed to these scores?

acyclic

Horsepower vs. MPG Grade:  $78\% \rightarrow \mathbf{B}$ 

acyclic

Altitude vs. Temperature Grade:  $43\% \rightarrow \mathbf{F}$ 

What contributed to these scores?

- acyclic
- Gaussian

Horsepower vs. MPG Grade:  $78\% \rightarrow \mathbf{B}$ 

acyclic

non-Gaussian

Altitude vs. Temperature Grade:  $43\% \rightarrow \mathbf{F}$ 

What contributed to these scores?

- acyclic
- Gaussian
- nonlinear

Horsepower vs. MPG Grade:  $78\% \rightarrow \mathbf{B}$ 

- acyclic
- non-Gaussian
- nonlinear

#### Real world data

Ground truth: Altitude → Temperature

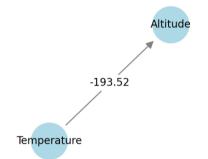


Figure 13: DirectLiNGAM prediction: altitude vs. temperature dataset

Ground truth: Horsepower → MPG

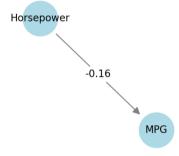


Figure 14: DirectLiNGAM prediction: horsepower vs. mpg dataset

# Wine Quality

Grade:  $78\% \rightarrow \mathbf{B}$ 

# Wine Quality

Grade:  $78\% \rightarrow B$ 

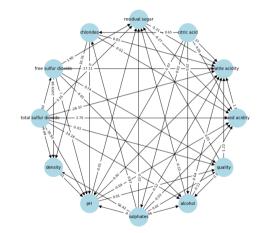


Figure 15: DirectLiNGAM prediction: wine quality dataset

# Wine Quality

Grade:  $78\% \rightarrow \mathbf{B}$ 

What contributed to this score?

- acyclic
- non-Gaussian
- nonlinear

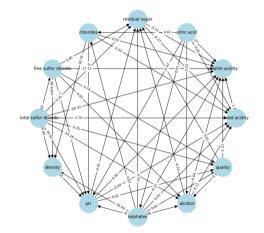


Figure 15: DirectLiNGAM prediction: wine quality dataset

Discoverability

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Conditional discovery

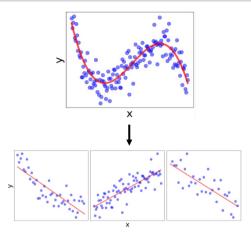


Figure 16: Nonlinear becomes linear with conditions

- Conditional discovery
- Existing literature



Figure 16: Relevant papers [8, 9, 10, 11]

Conditional discovery

- Existing literature
- Choosing an algorithm

- Peter-Clark Algorithm
- Inductive Causation Algorithm
- Fast Causal Inference Algorithm
- ICA-LiNGAM
- Pairwise LiNGAM

Table 7: Some other causal discovery algorithms [12, 13]

- Conditional discovery
- Existing literature

- Choosing an algorithm
- Machine learning

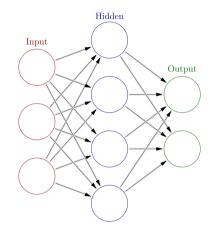


Figure 16: Find a neural net picture

- Conditional discovery
- Existing literature
- Choosing an algorithm
- Machine learning

Interface

Complete: front-end of interface

Complete: front-end of interface

Incomplete: integration

Complete: front-end of interface

Incomplete: integration



Figure 16: Welcome screen



Figure 17: Upload data



Figure 18: Reliability score

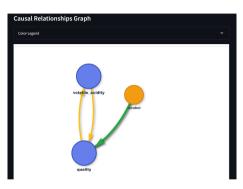


Figure 19: Causal graph

### Conclusion

How can we enhance discoverability with modern causal AI?

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How can we enhance discoverability with modern causal AI?

We can enhance discoverability with modern causal AI by establishing clear metrics for reliability.

### The End

Questions?

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- Initialize:
  - x: a p-dimensional random vector
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  - $\circ$  Find  $x_m$ : the most independent variable

$$x_m = \arg\min_{j \in U \setminus K} T_{kernel}(x_j; U \setminus K)$$

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- **4** Construct lower triangular matrix, B, estimating connection strengths,  $b_{ij}$ , using covariance-based regression. (LS or MLE)

Discoverability

```
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Let predictor variables x_1, \dots, x_p \in \mathbf{R}^{n \times 1}, where X = [x_1 \dots x_p],
```

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Observe:

$$Y = X\beta$$

$$X^{T}Y = X^{T}X\beta$$

$$(X^{T}X)^{-1}X^{T}Y = \beta$$

Thus, we have found the coefficients, i.e.,  $\beta$ .