

# Learning causal DAGs using adaptive interventions

Davin Choo

24 Feb 2023

Computing Research Week - Open House 2023

This talk is based on joint work with  
Arnab **B**hattacharyya, Themis **G**ouleakis, Kirankumar **S**hiragur



# Important decisions in life...

- **What if** I ate Kaya Toast instead of Roti Prata for breakfast? Will I feel more satisfied?



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- **What if** I exercised more? Will I become fitter?
- **What if** I went to University X instead of NUS? Will I be more successful?
- ...



# Important decisions in life...

- **What if** I ate Kaya Toast instead of Roti Prata for breakfast? Will I feel more satisfied?



- **What if** I exercised more? Will I become fitter?
- **What if** I went to University X instead of NUS? Will I be more successful? **Not necessarily. We have great people here 😊**
- ...



David Hume  
Philosopher

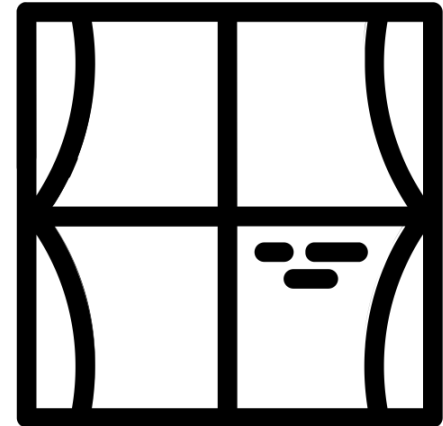
One of his philosophical ideas:

- To draw any causal conclusions from past experiences, one has to assume that the future resembles the past
- This assumption cannot be justified



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Yesterday

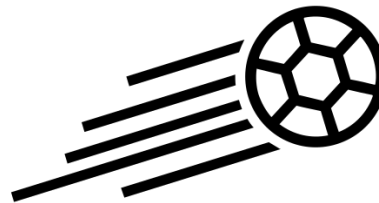


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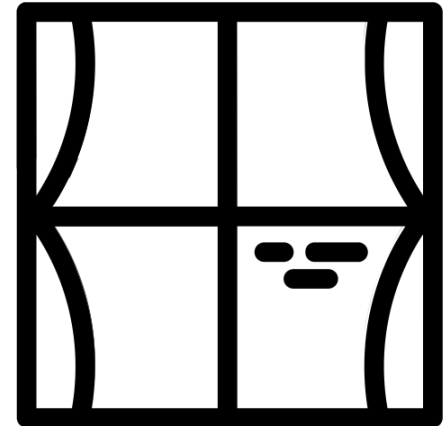
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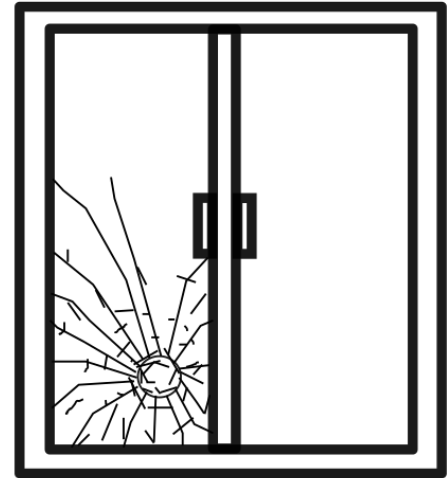
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Did the ball smash the  
window?

OR

Did the smashed window  
summon the ball?



Da  
Ph

To make useful causal conclusions,  
make useful/reasonable model  
assumptions or conduct experiments

One of

- To draw conclusions from past experiences, one has to assume that the future resembles the past
- This assumption cannot be justified

Today



h the

OR

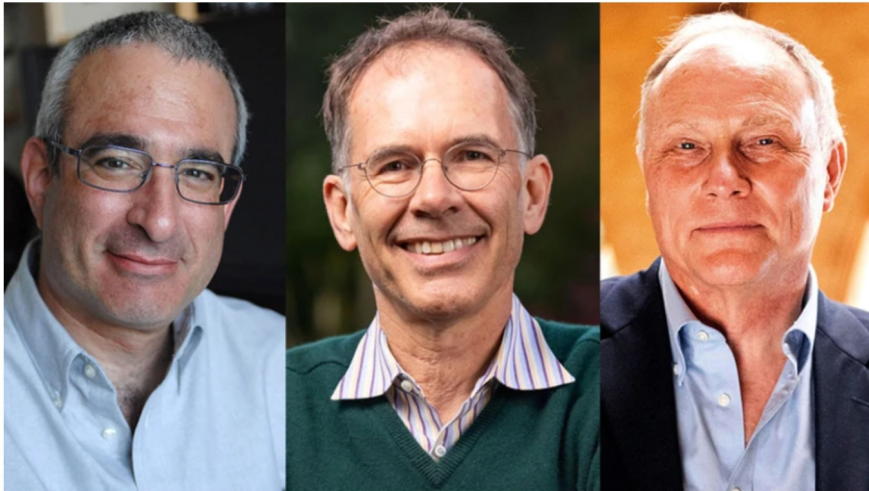
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NEWS | 13 October 2021

# Nobel-winning 'natural experiments' approach made economics more robust

Joshua Angrist, Guido Imbens and David Card share the prize for finding a way to identify cause and effect in social science.

Philip Ball 



Left to Right: Joshua Angrist, Guido Imbens and David Card share the 2021 Nobel prize in economic sciences for work that has helped economics research undergo a 'credibility revolution'. Credit: MIT/EPA-EFE/Shutterstock, Andrew Brodhead/Stanford News Service/EPA-EFE/Shutterstock, Noah Berger/AP/Shutterstock

NEWS | 13 October 2021

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**JUDEA PEARL** 

United States - 2011

(2011 Turing award)

CITATION

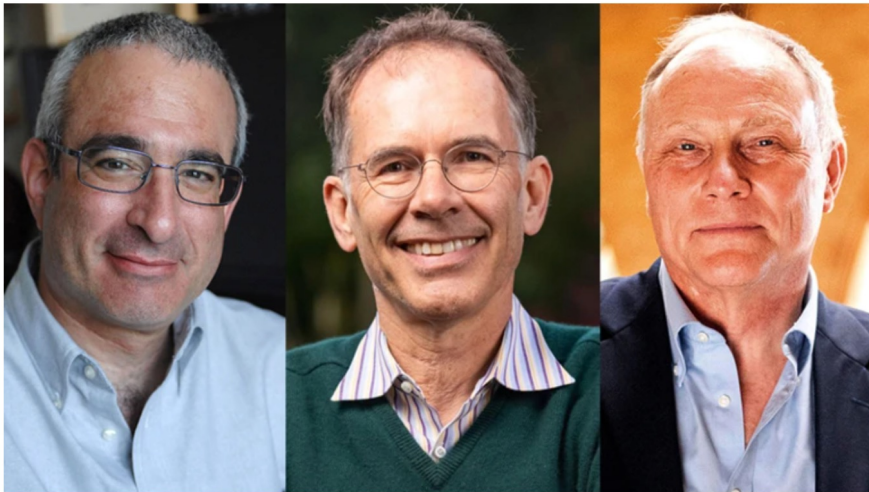
For fundamental contributions to artificial intelligence through the development of a calculus for probabilistic and causal reasoning.

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## JUDEA PEARL

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### CITATION

For fundamental contributions to artificial intelligence through the development of a calculus for probabilistic and causal reasoning.

- Bayesian networks
  - Represent causal relationships as a directed acyclic graph (DAG)
- Do-calculus
  - A formalization of interventions
  - “What happens if we perform experiments on the causal graph?”



# Modelling causal relations

**“We may regard the present state of the universe as the effect of its past and the cause of its future...”** – Pierre Simon Laplace,  
*A Philosophical Essay on Probabilities*, 1814



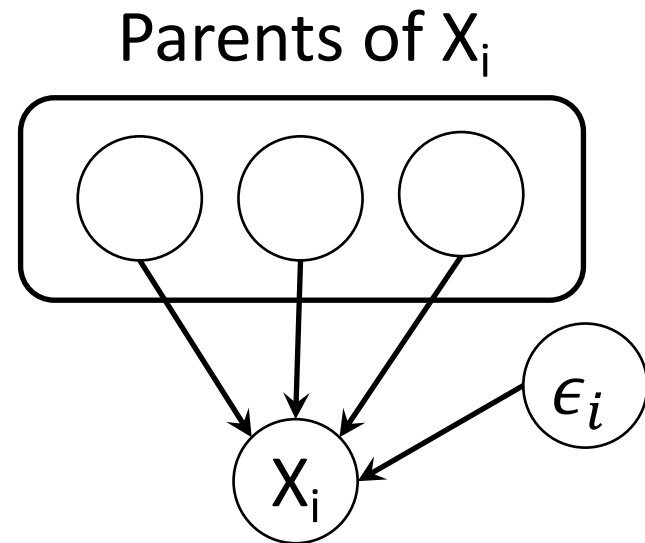
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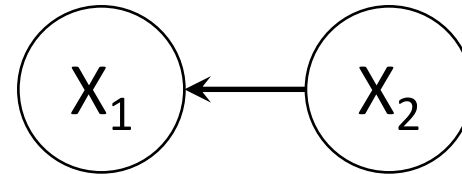
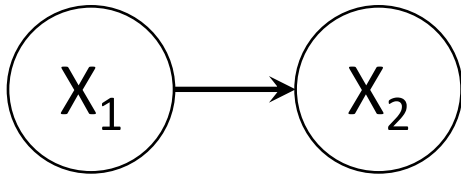
$$X_i = f_i(pa_i, \epsilon_i)$$

The value of each variable  $X_i$  is function  $f_i$  of the values taken by its parents  $pa_i$  and some noise  $\epsilon_i$



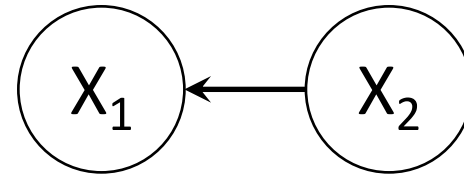
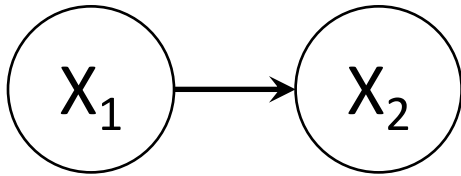
# Which model generated this data?

$X_1$	-0.27	0.29	0.37	-0.09	0.34	0.33	0.30	-1.34	0.68
$X_2$	-0.10	1.65	0.47	1.92	2.04	1.67	0.11	-3.58	1.97



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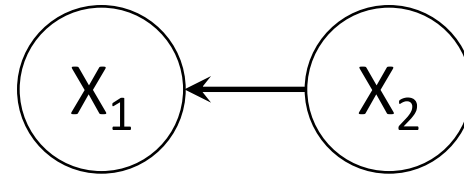
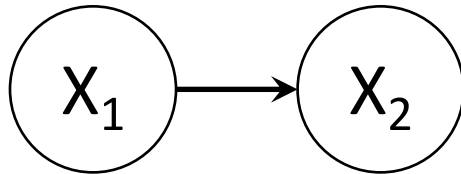
- $X_1 = \epsilon_1$
- $X_2 = a \cdot X_1 + \epsilon_2$

- $X_1 = b \cdot X_2 + \epsilon_3$
- $X_2 = \epsilon_4$

Simple linear relationship between variables  
a and b are (hidden) positive constants  
 $\epsilon$ 's are independent Gaussian terms with mean 0

# Two equivalent causal models

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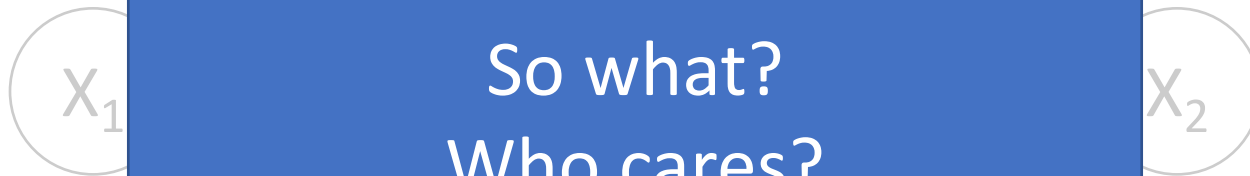


- $X_1 = \epsilon_1 \sim N(0, 1)$
- $X_2 = X_1 + \epsilon_2 \sim N(0, 2)$
- $\epsilon_1 \sim N(0, 1)$
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- $X_1 = \frac{1}{2} \cdot X_2 + \epsilon_3 \sim N(0, 1)$
- $X_2 = \epsilon_4 \sim N(0, 2)$
- $\epsilon_3 \sim N\left(0, \frac{1}{2}\right)$
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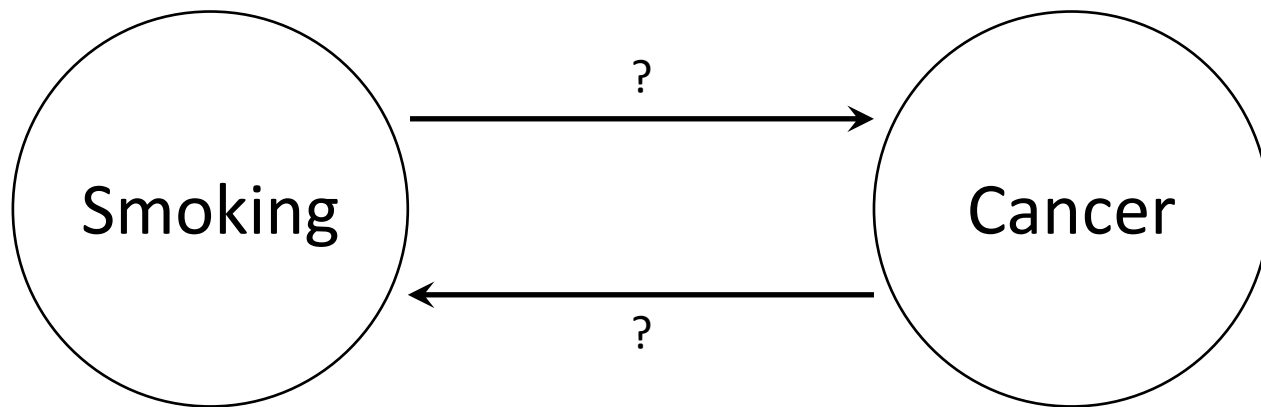


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# Smoking

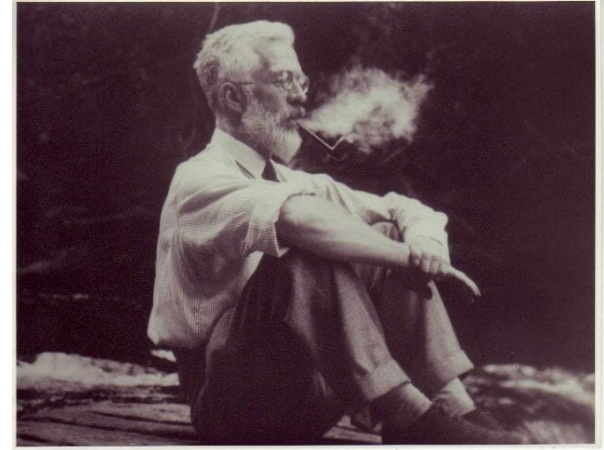
<b>Smoking</b>	Yes	Yes	Yes	No	No	No	...
<b>Cancer</b>	No	Yes	Yes	No	No	Yes	...



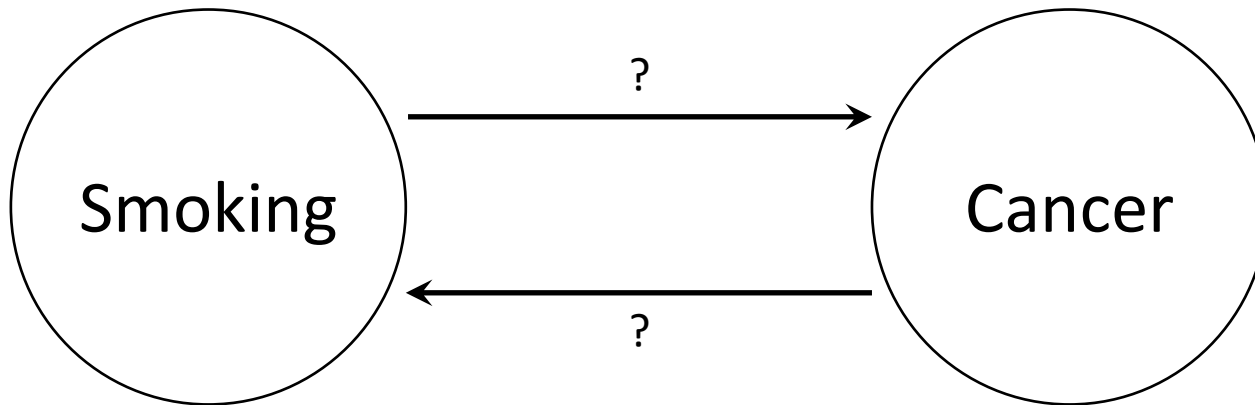
# Smoking

Fisher's letter to Nature, 1958:

"The curious associations with lung cancer found in relation to smoking habits do not, in the minds of some of us, lend themselves easily to the simple conclusion that the products of combustion reaching the surface of the bronchus induce, though after a long interval, the development of a cancer... **Such results suggest that an error has been made, of an old kind, in arguing from correlation to causation...**"



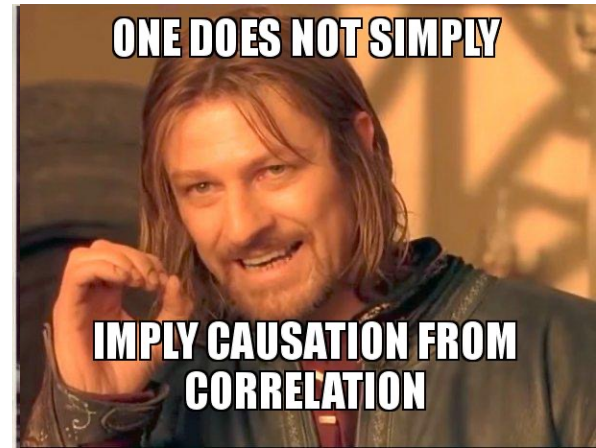
Ronald Fisher



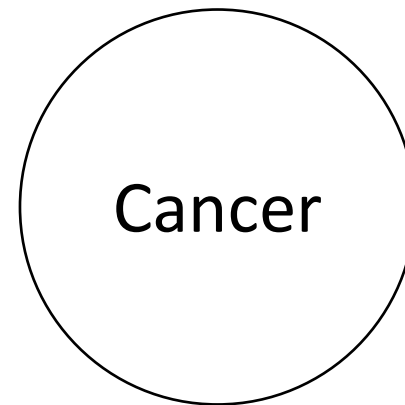
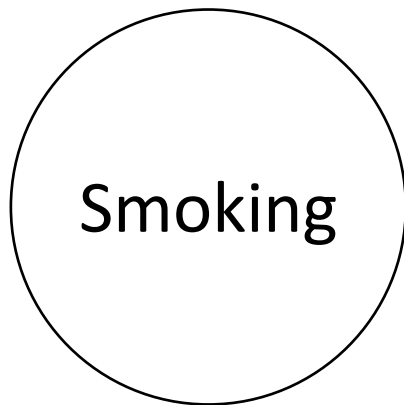
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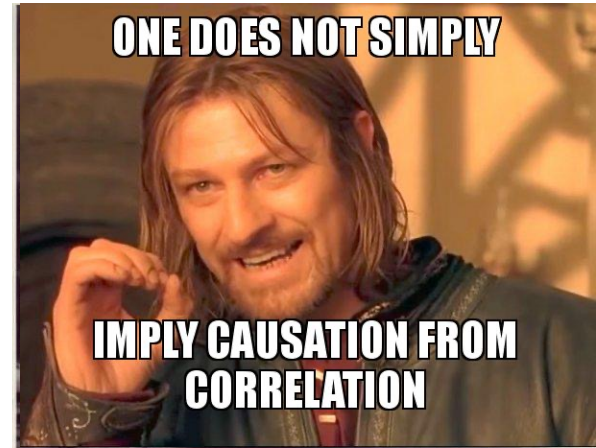
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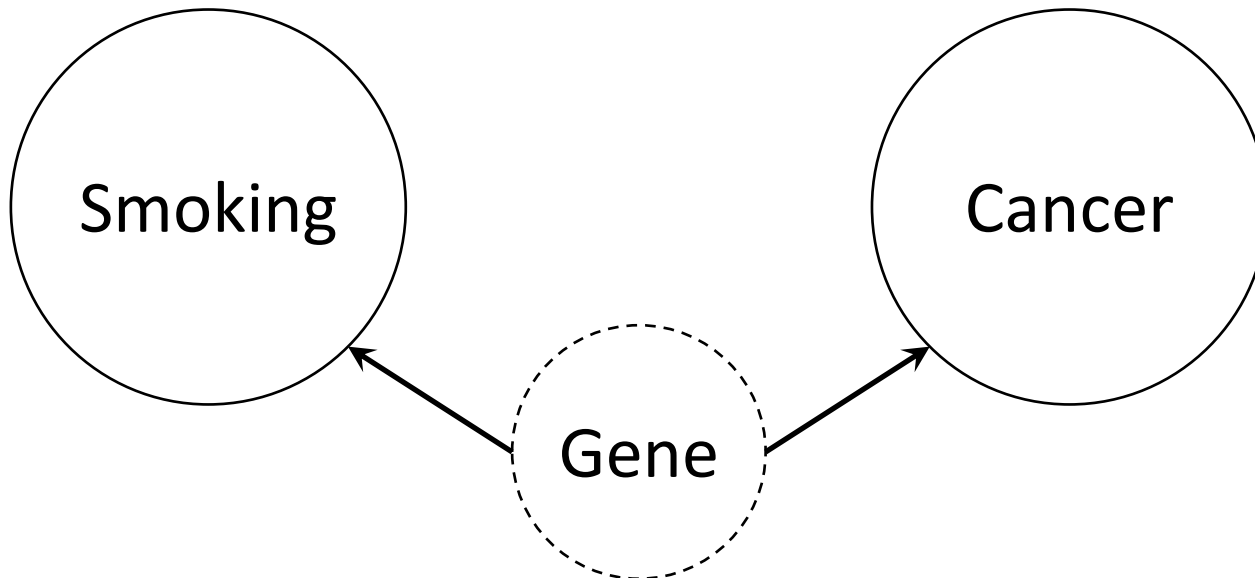
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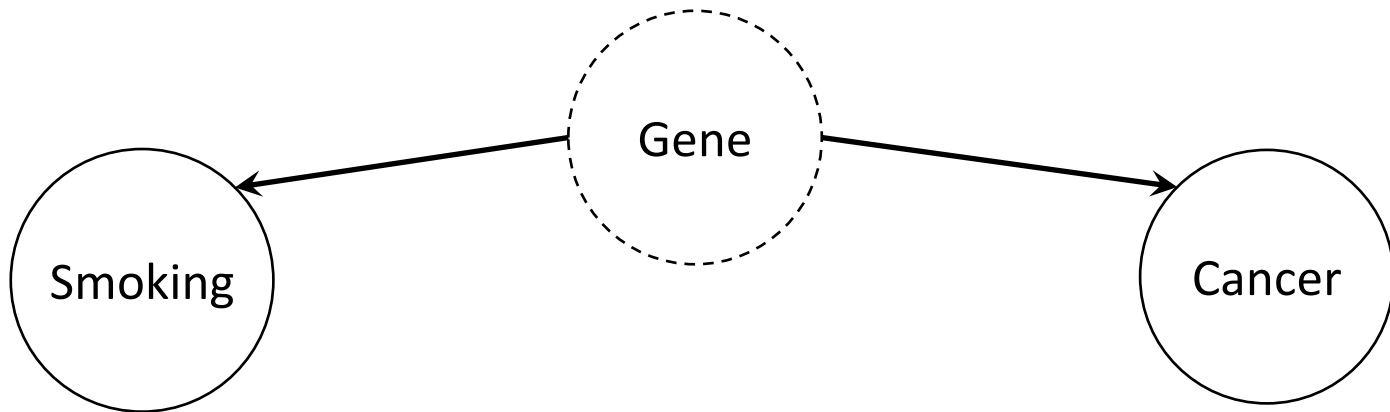
"... Such results suggest that an error has been made, of an old kind, in arguing from correlation to causation, and that the possibility should be explored that the different smoking classes, non-smokers, cigarette smokers, cigar smokers, pipe smokers, etc., have adopted their habits partly by reason of their personal temperaments and dispositions, and are not lightly to be assumed to be equivalent in their **genotypic composition**..."



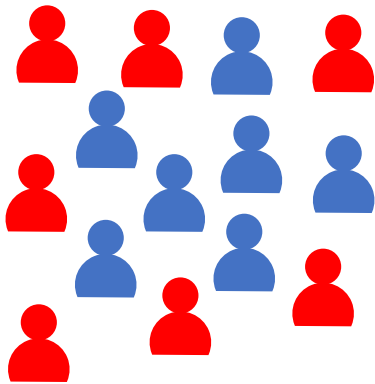
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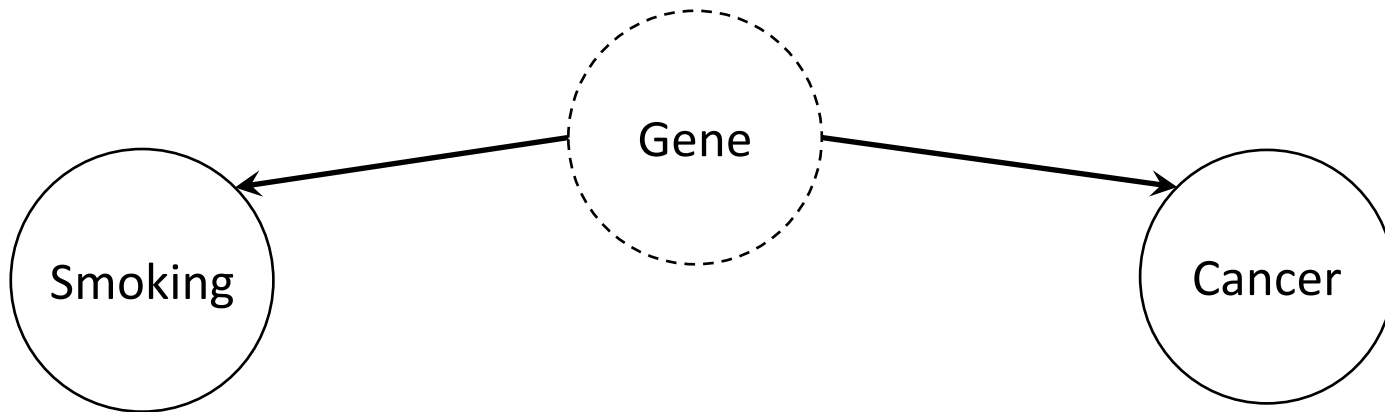


Maybe there's an unmeasured confounder?

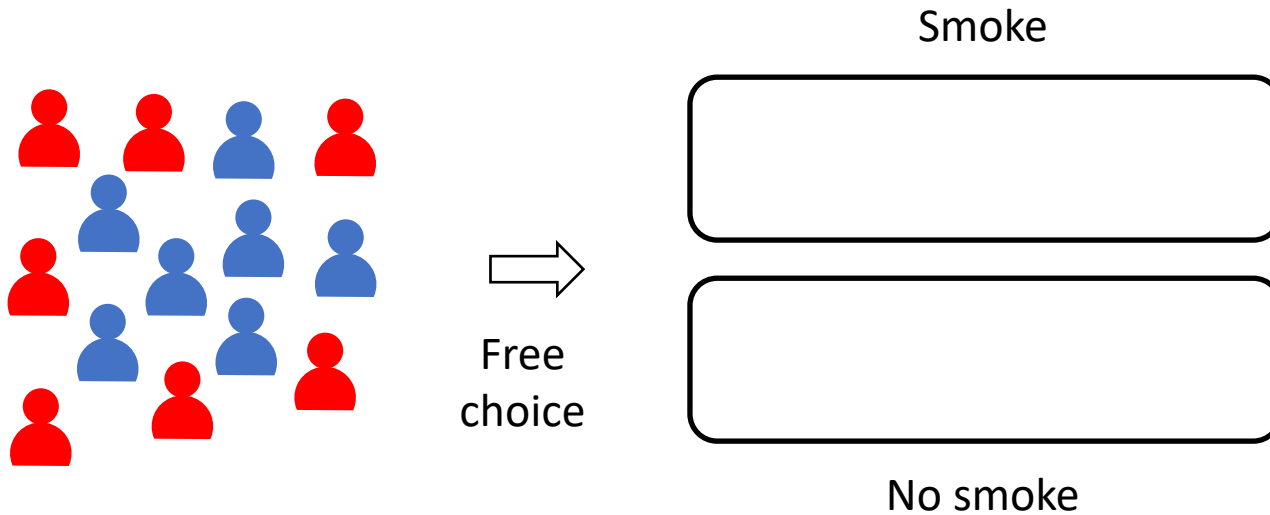


Hypothesis: There are two types of people in the world

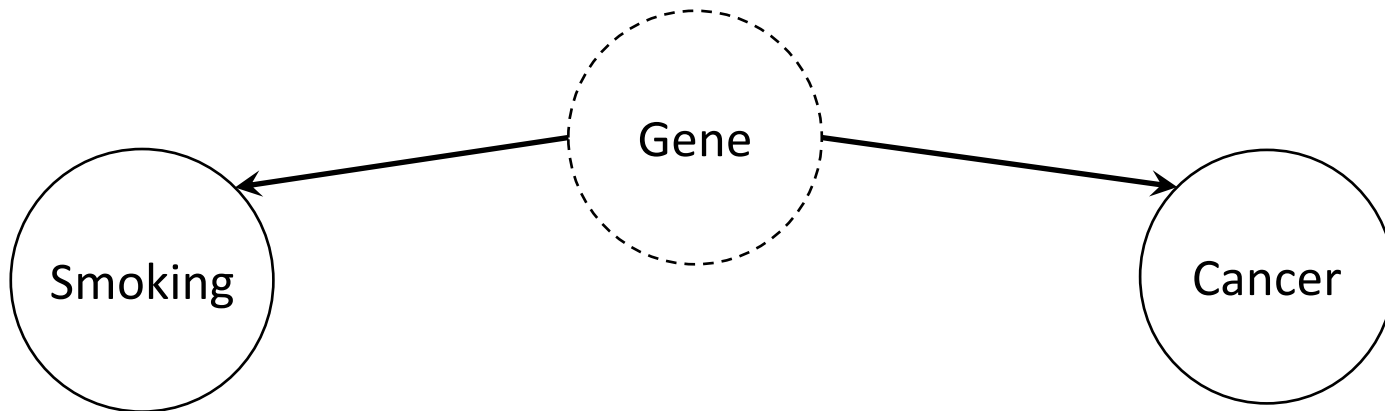




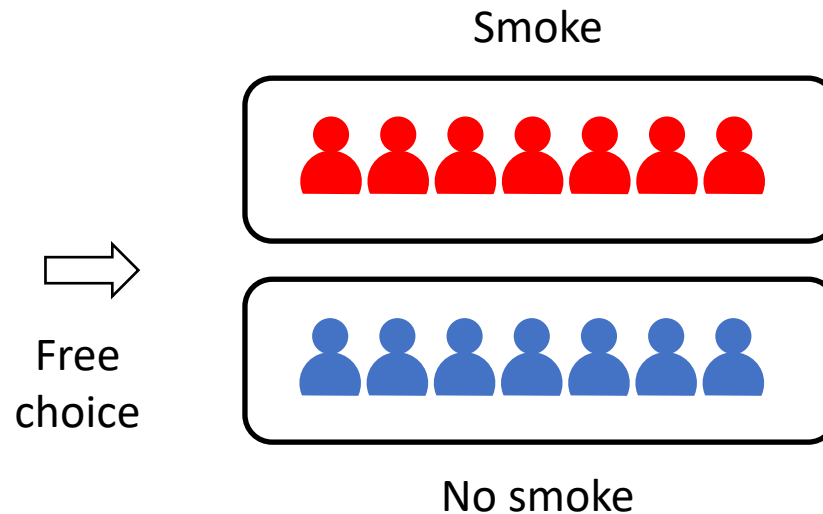
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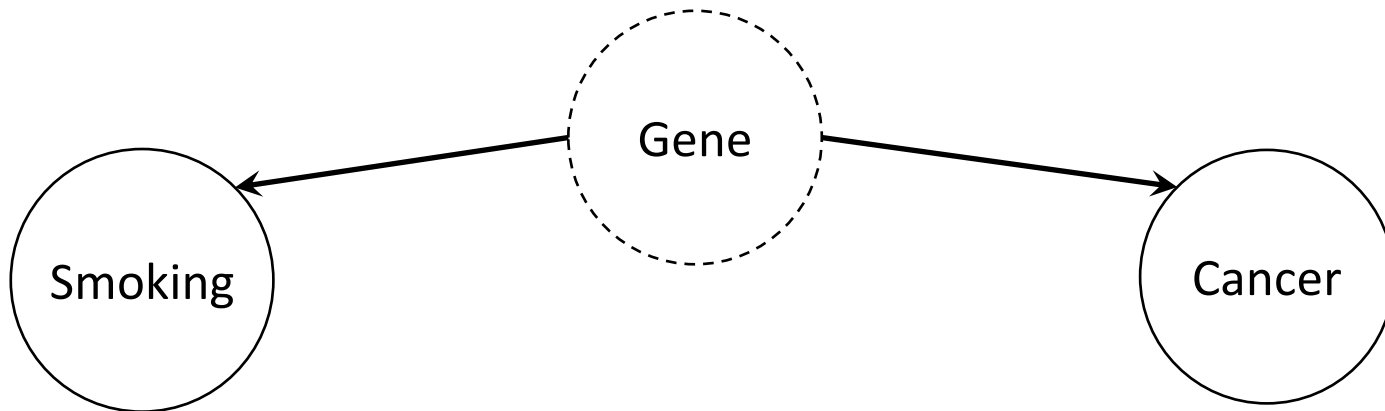




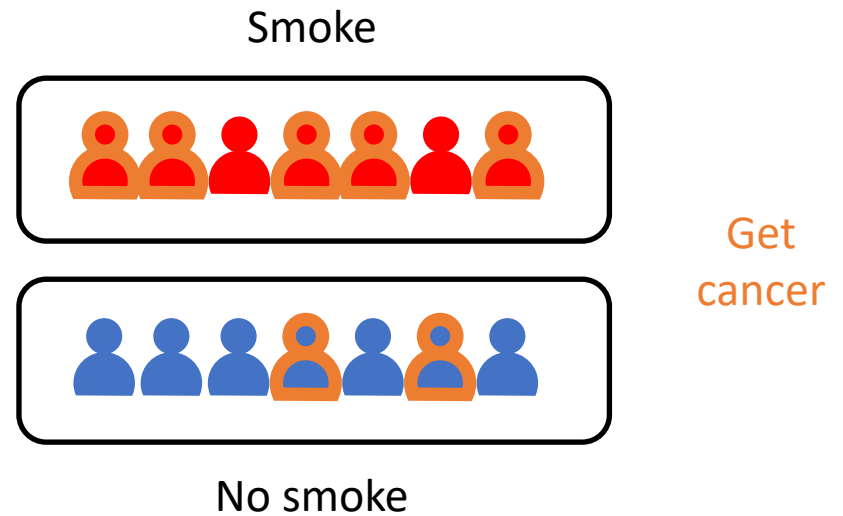


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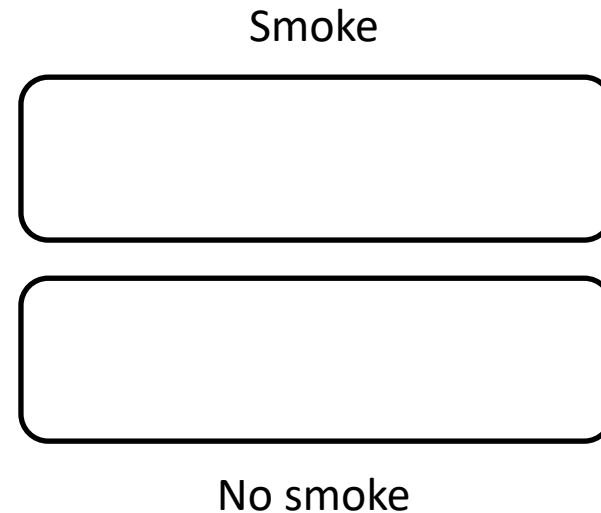
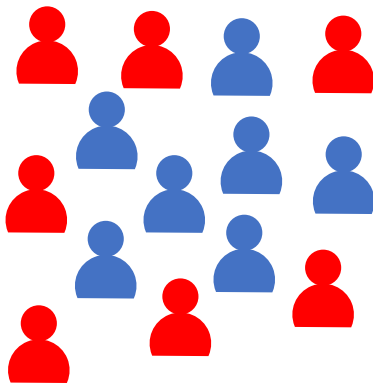


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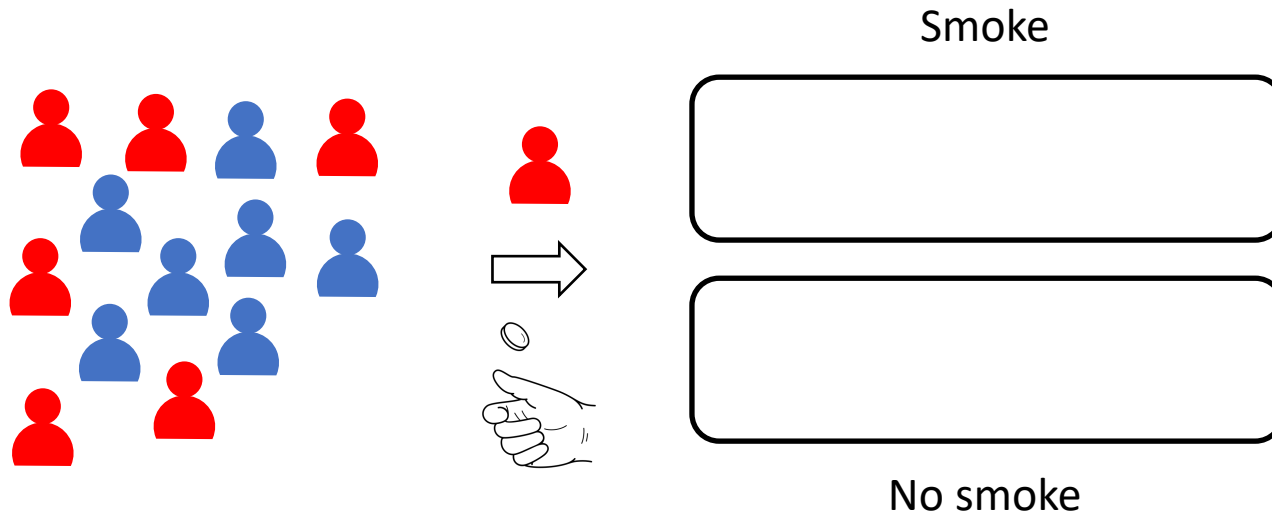
# Randomized controlled trials

- Gold standard in scientific exploration
- RCTs  $\equiv$  Interventions in causality



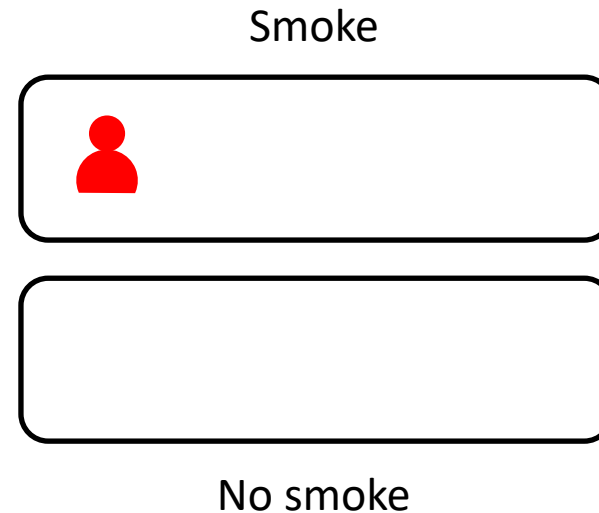
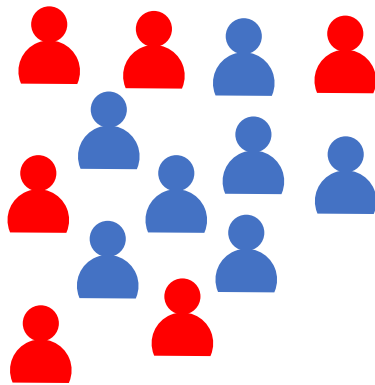
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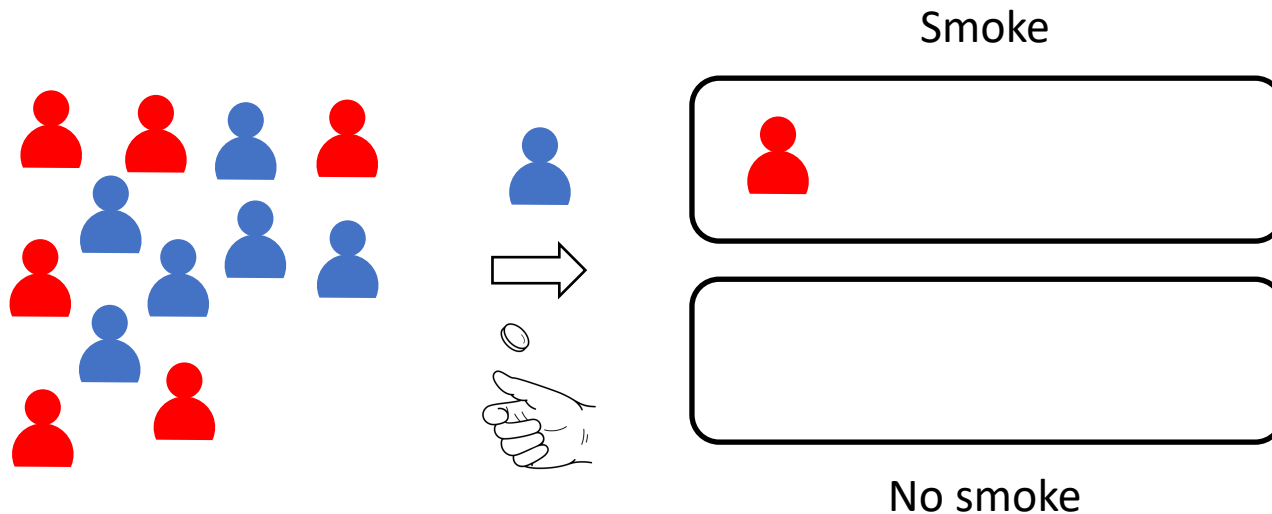
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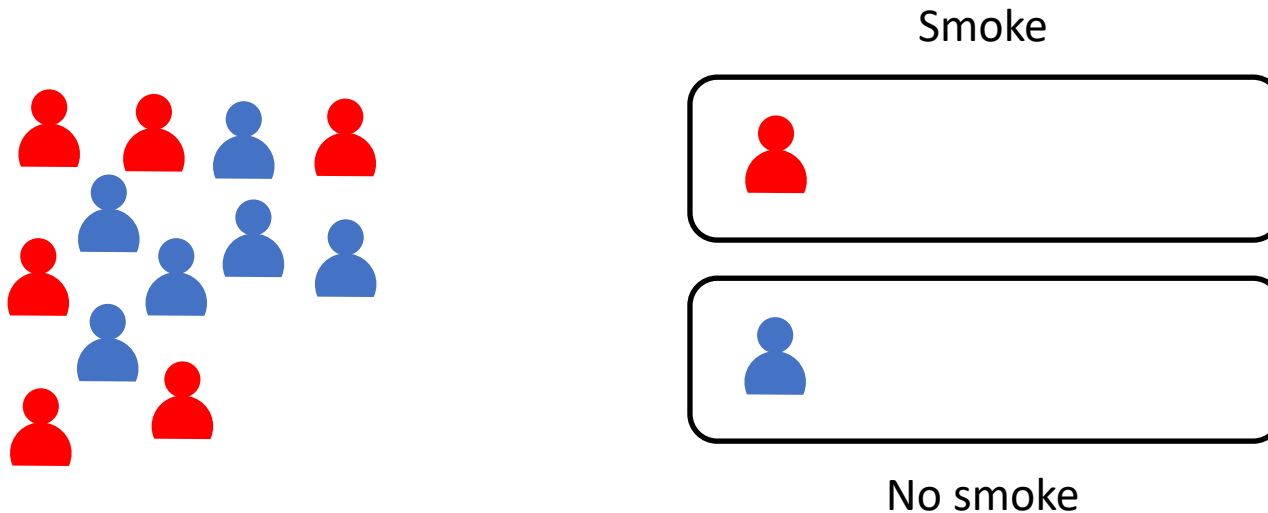
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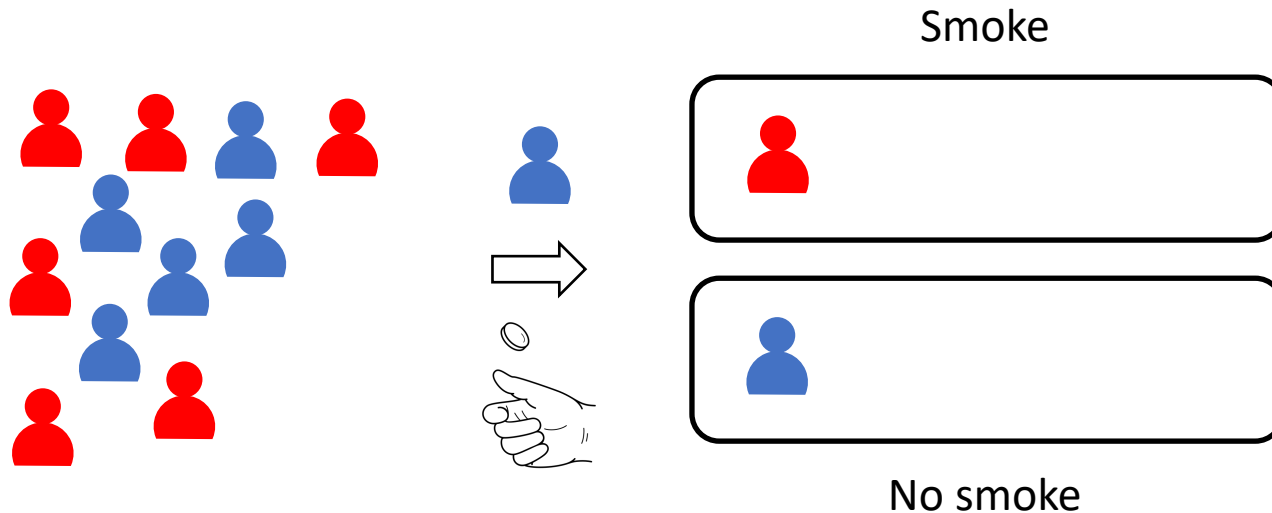
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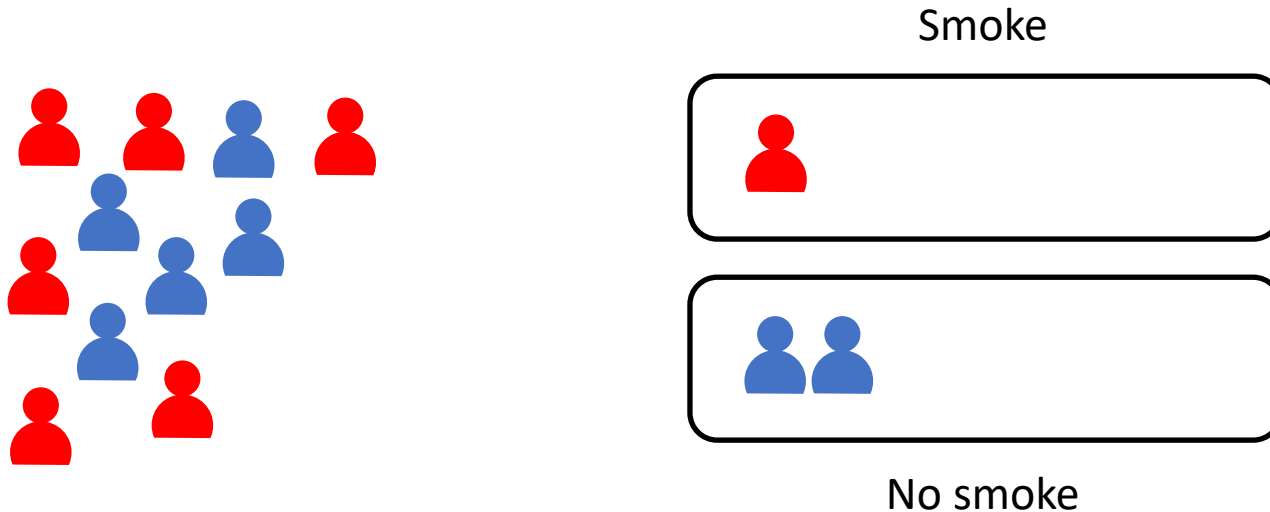
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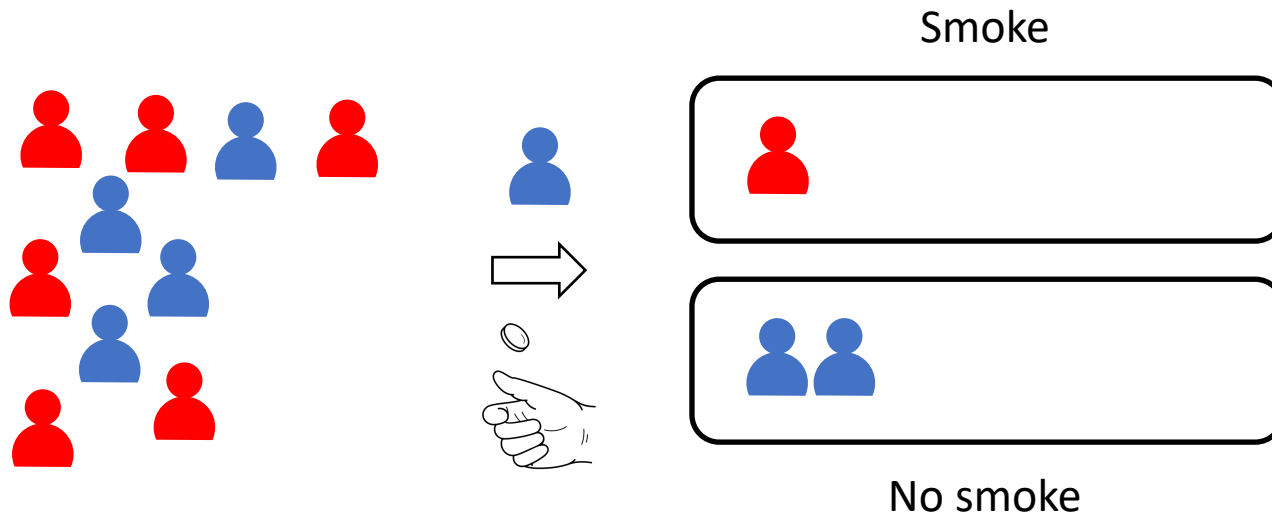
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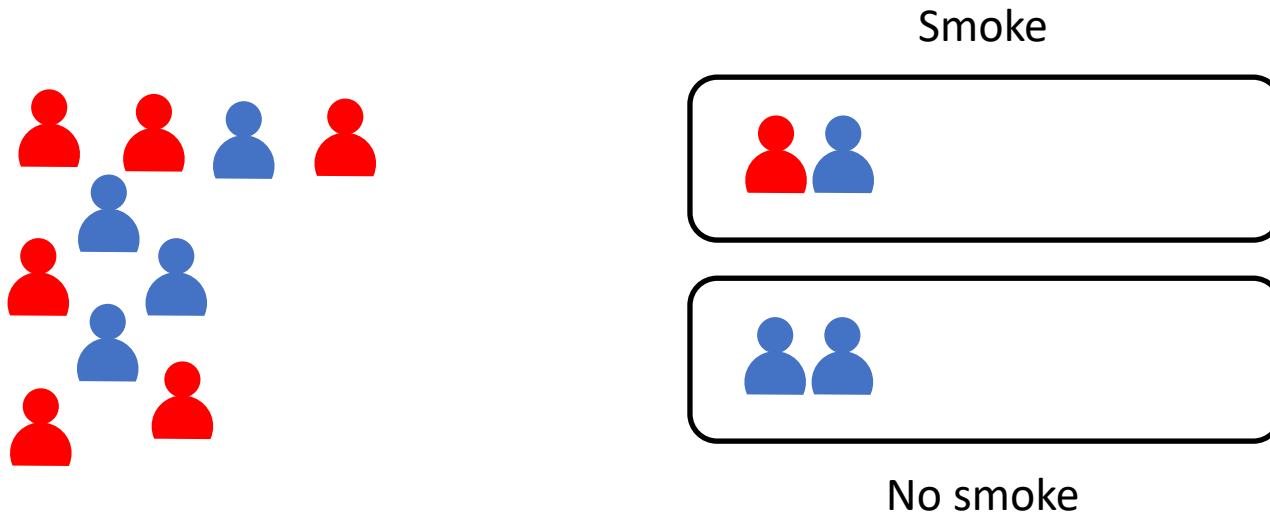
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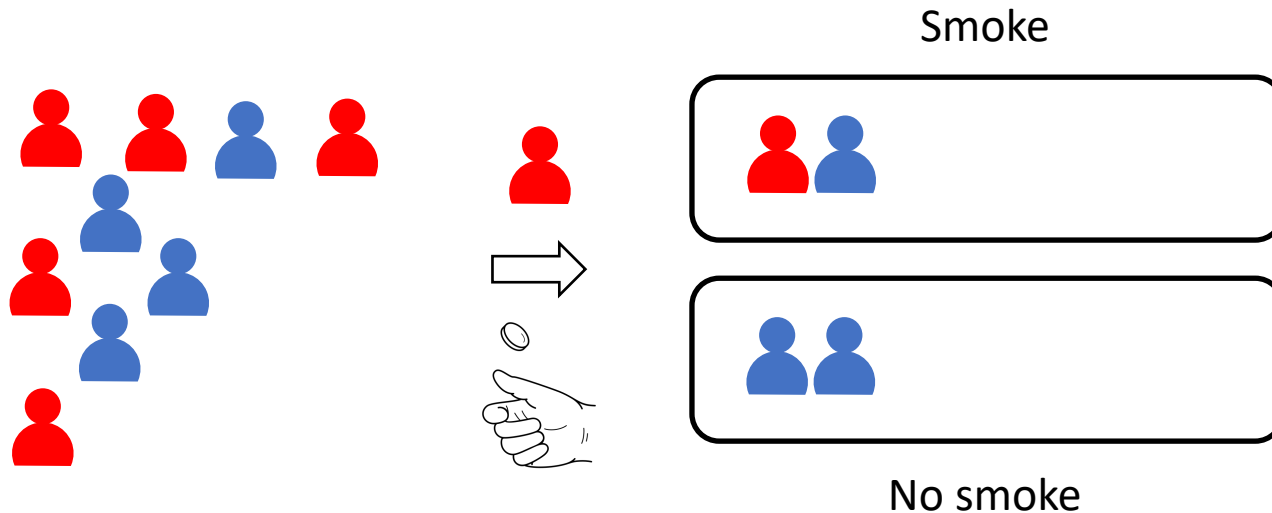
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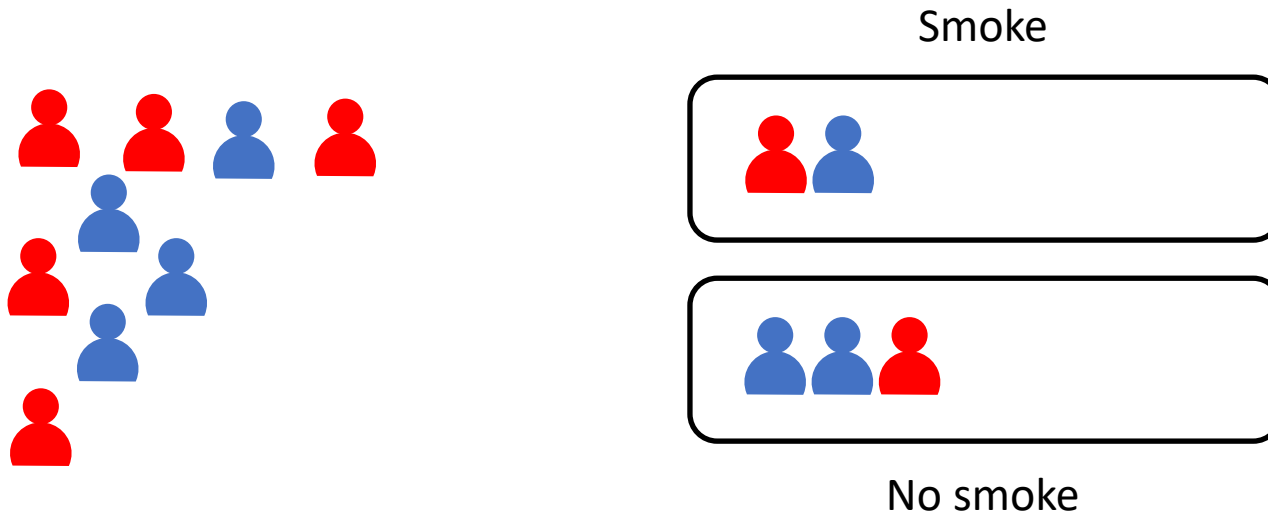
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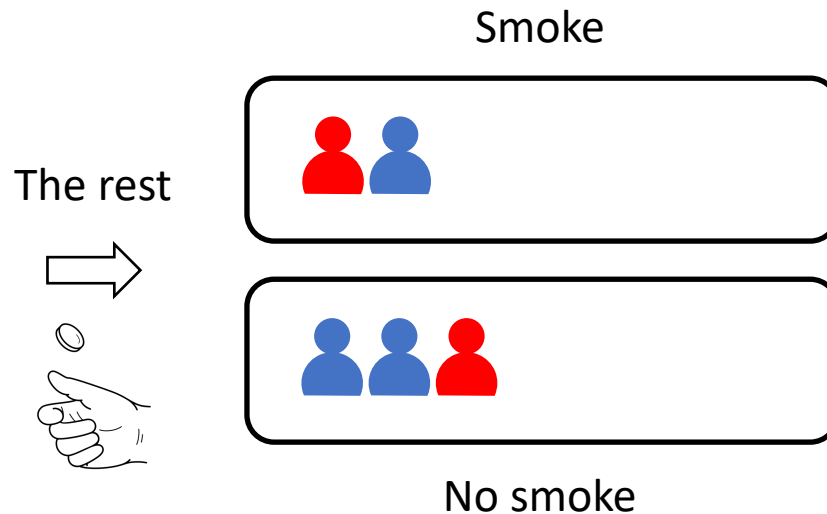
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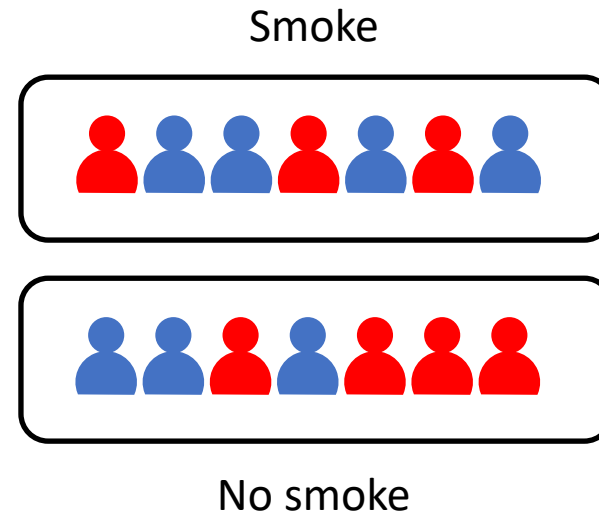
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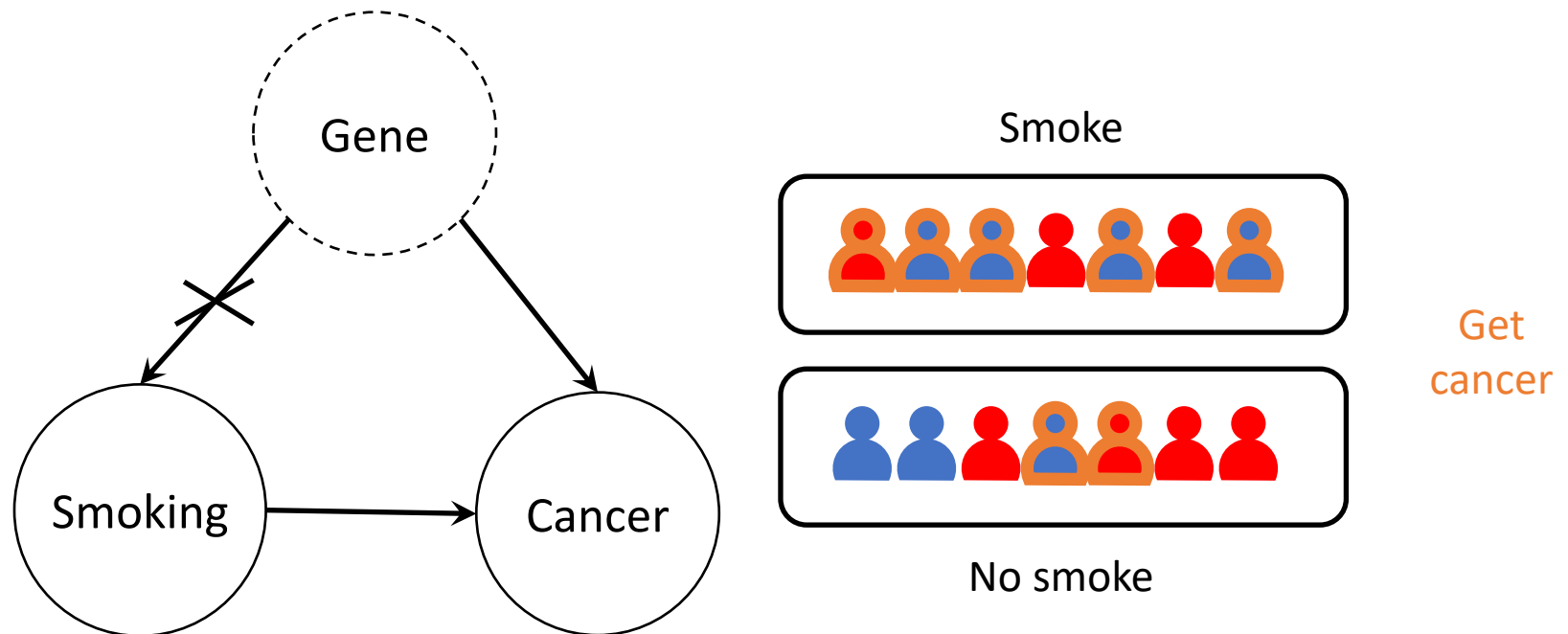
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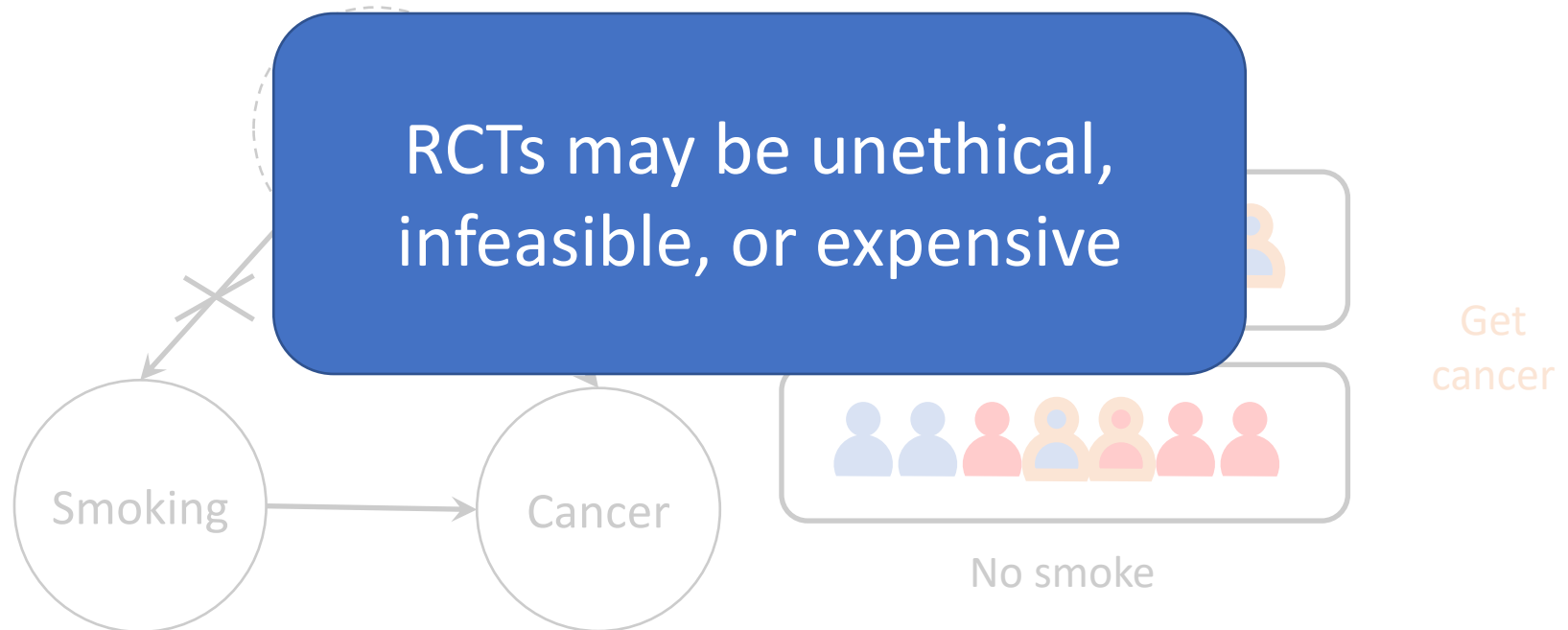


RCT removed causal link from “gene” to “smoking”

If smoking and cancer still highly correlated, then smoking causes cancer

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If smoking and cancer still highly correlated, then smoking causes cancer



ERIC AND WENDY  
SCHMIDT CENTER  
AT BROAD INSTITUTE

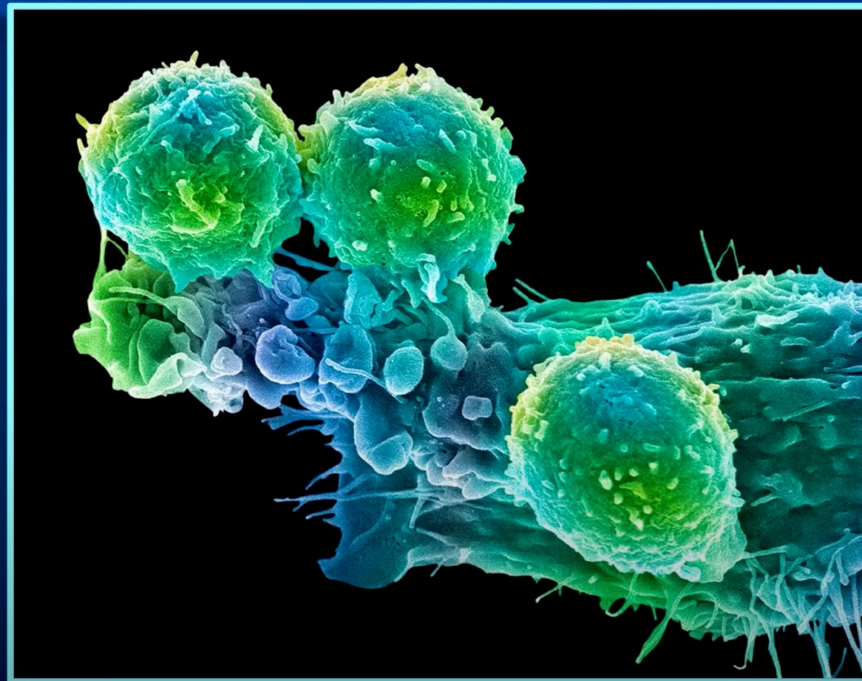
# CANCER IMMUNOTHERAPY DATA SCIENCE GRAND CHALLENGE

2023

☰ Lecture 1, Biology: Section B

Press `esc` to exit full screen

## T cells attacking a cancer cell



Janeway Immunology  
Image by Steve  
Gschmeissner/Science Photo Library

⏪ ⏩ ⏴ ⏵ 2:50 / 3:31



Lecture 1, Biology: Section C

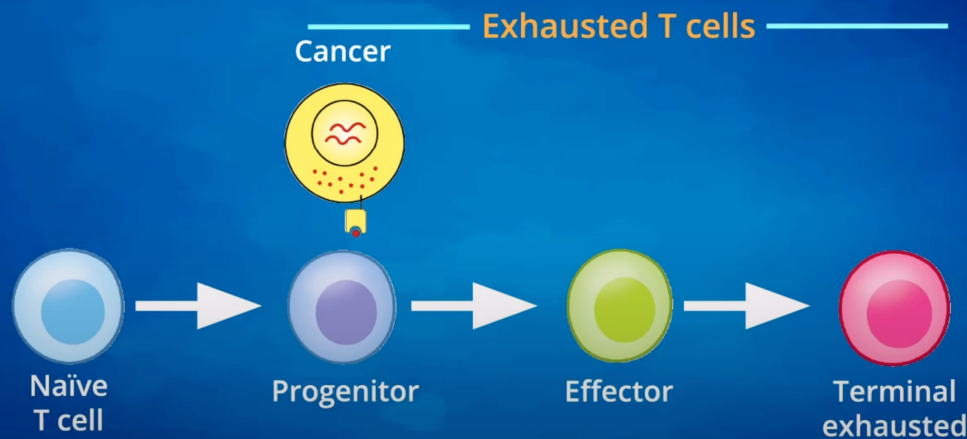
## Cancer evades T cell killing by driving T cells to exhaustion.



Site:

Blood

Tumor



T cell states are encoded by gene expression programs, which change upon encounter with cancer cells.

0:58 / 5:09

CC BY ND



## Cancer immunotherapies only work for some people and for some cancer types



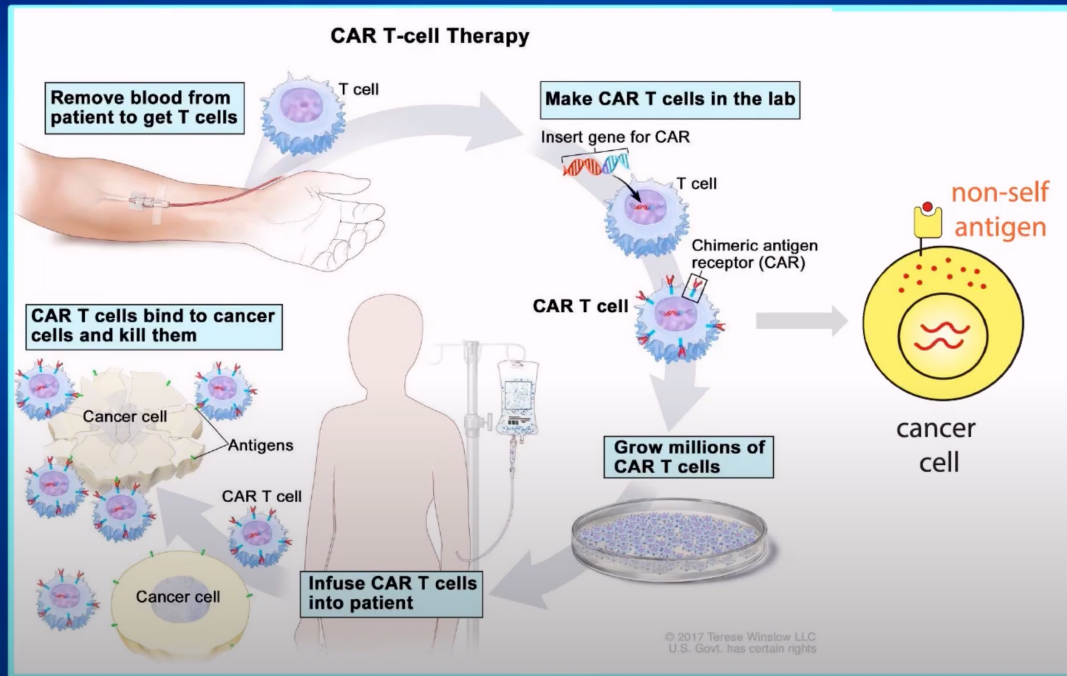
- Cancer cells do not act through PD-1 or CTLA-4.
- Cancer cells directly inhibit T cells through a new signaling pathway.
- Cancer cells indirectly inhibit T cells by creating a suppressive immune environment.
- CAR T cell exhaustion.
- And more...
- [clinicaltrials.gov](https://clinicaltrials.gov): 2500 studies found for *Immune checkpoint inhibitor* and 1000 studies found for CAR T cell

Challenge opportunity  
What other genetic changes in T cells would make them better cancer killers?

Lecture 1, Biology: Section D

Press `esc` to exit full screen

## Cancer Immunotherapy: CAR T-cell therapy



Treating diffuse large B-cell lymphoma with CAR T cells.

- ~50% of treated patients have durable complete response.

cancer.gov

June, C. H. et al *New England Journal of Medicine* (2018)





ERIC AND WENDY  
SCHMIDT CENTER  
AT BROAD INSTITUTE

# CANCER IMMUNOTHERAPY DATA SCIENCE GRAND CHALLENGE

2023

Basically,

1. Take T-cell out of cancer patient
2. Perform **interventions** on T-cell genes, so that these cells are less likely to become exhausted
3. Put back into cancer patient

Ca

Rem  
patie

CAR T  
cells a

Cancer cell

Infuse CAR T cells  
into patient

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U.S. Govt. has certain rights

cancer.gov

June, C. H. et al *New England  
Journal of Medicine* (2018)



5:24 / 8:58





NEWS | 07 October 2020



# Pioneers of revolutionary **CRISPR** gene editing win chemistry Nobel

Emmanuelle Charpentier and Jennifer Doudna share the award for developing the **precise genome-editing technology.**

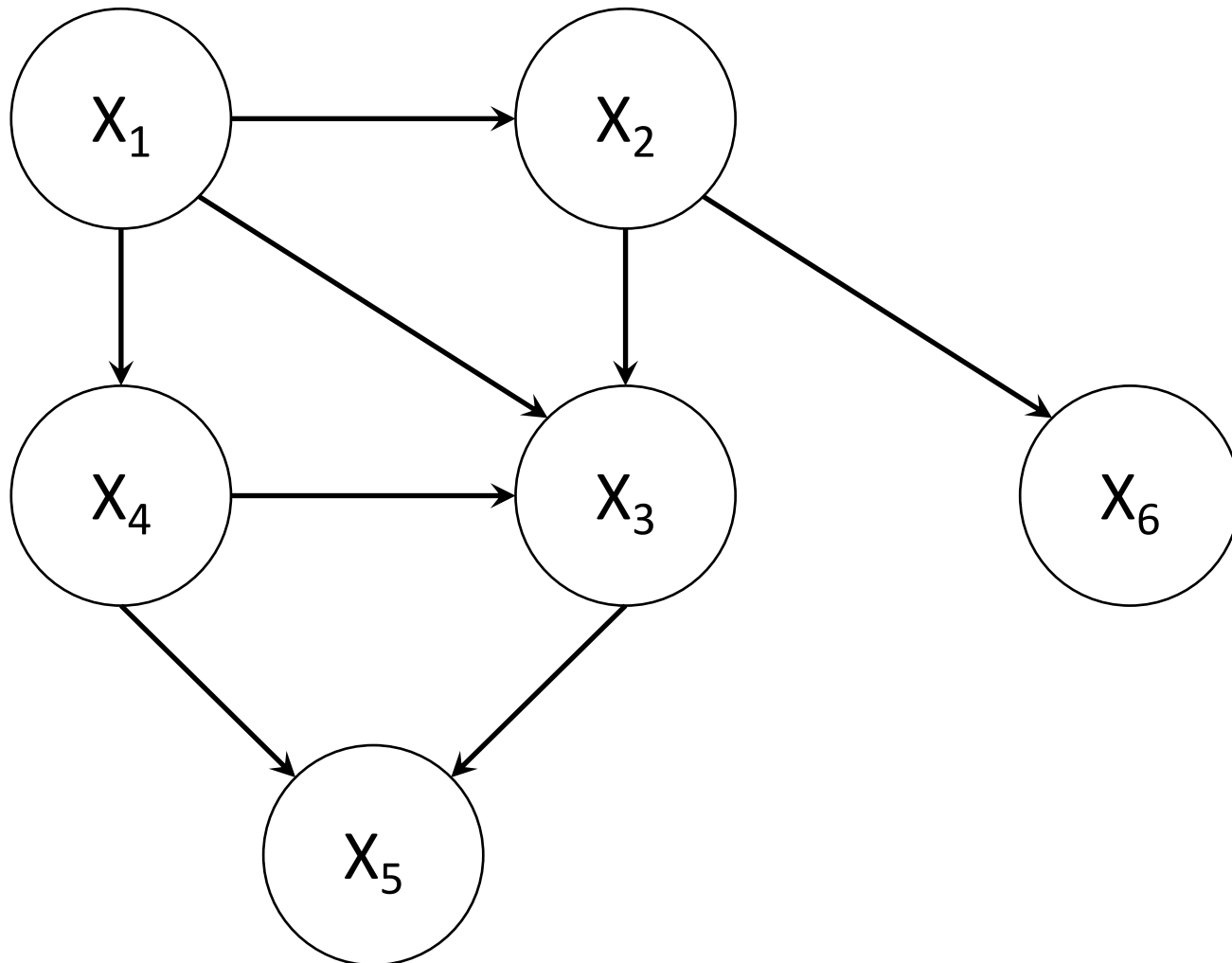
[Heidi Ledford](#) & [Ewen Callaway](#)



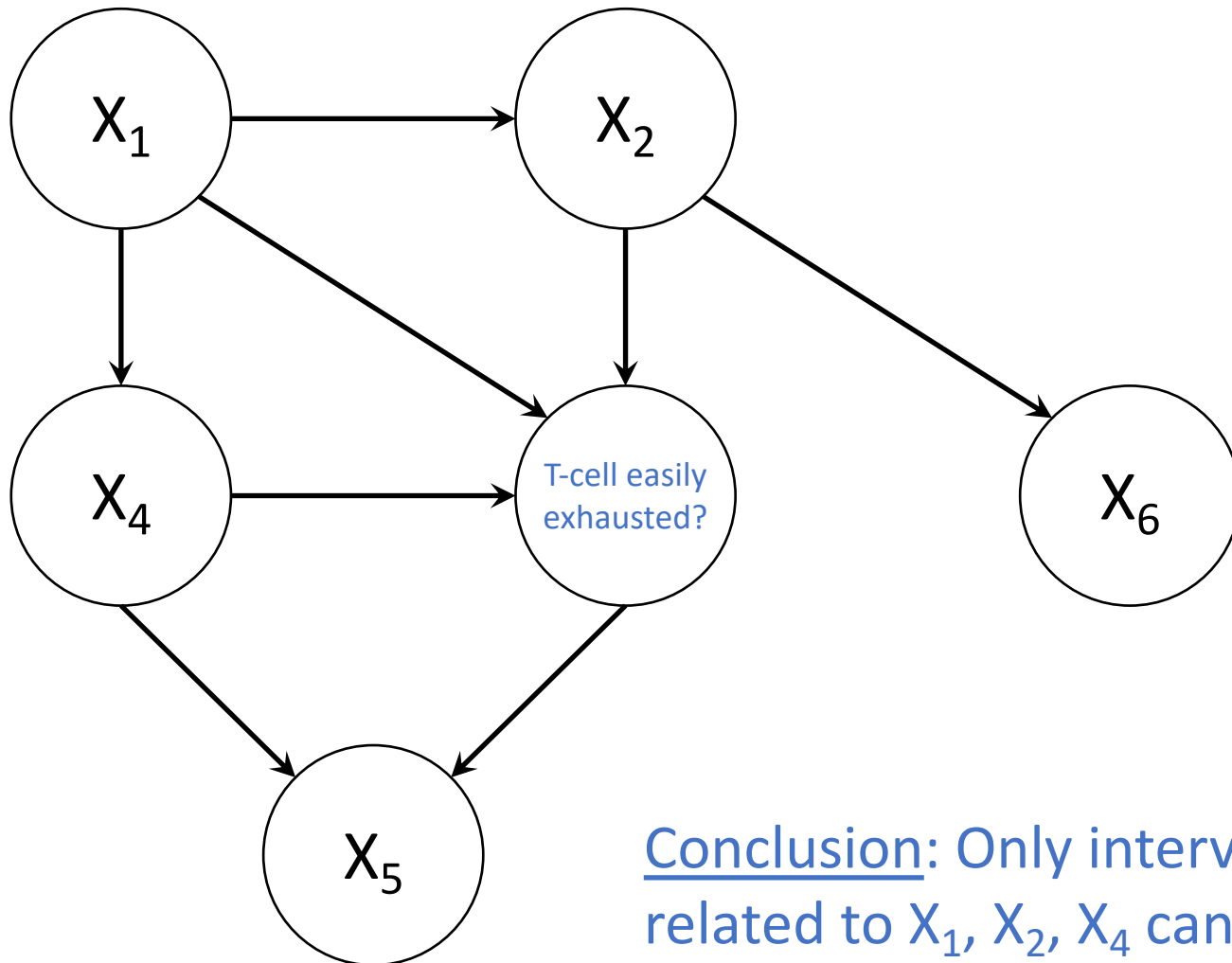
Jennifer Doudna and Emmanuelle Charpentier share the **2020 Nobel chemistry prize** for their discovery of a game-changing gene-editing technique. Credit: Alexander Heinel/Picture Alliance/DPA

- 1.
- 2.
- 3.

# Why structure learning



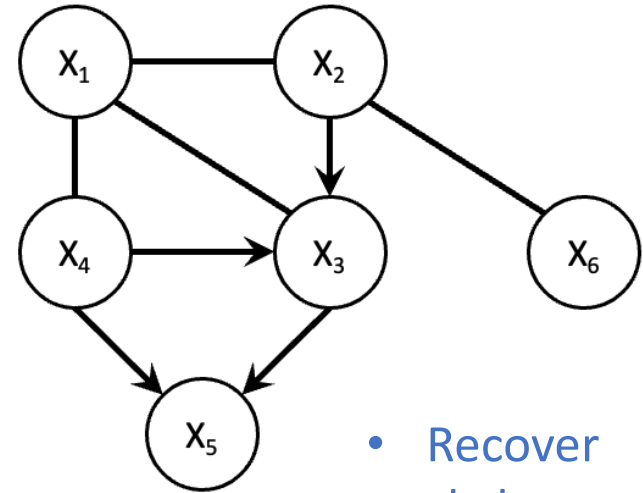
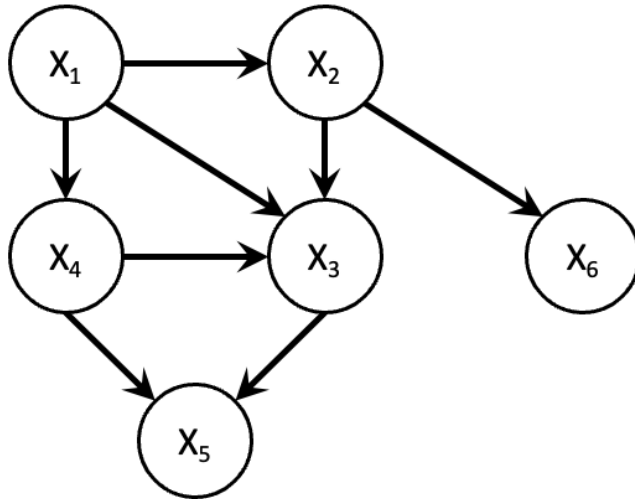
# Why structure learning



Conclusion: Only interventions related to  $X_1$ ,  $X_2$ ,  $X_4$  can affect our objective of interest

# Structure learning (simplified)

This represents an equivalence class of graphs

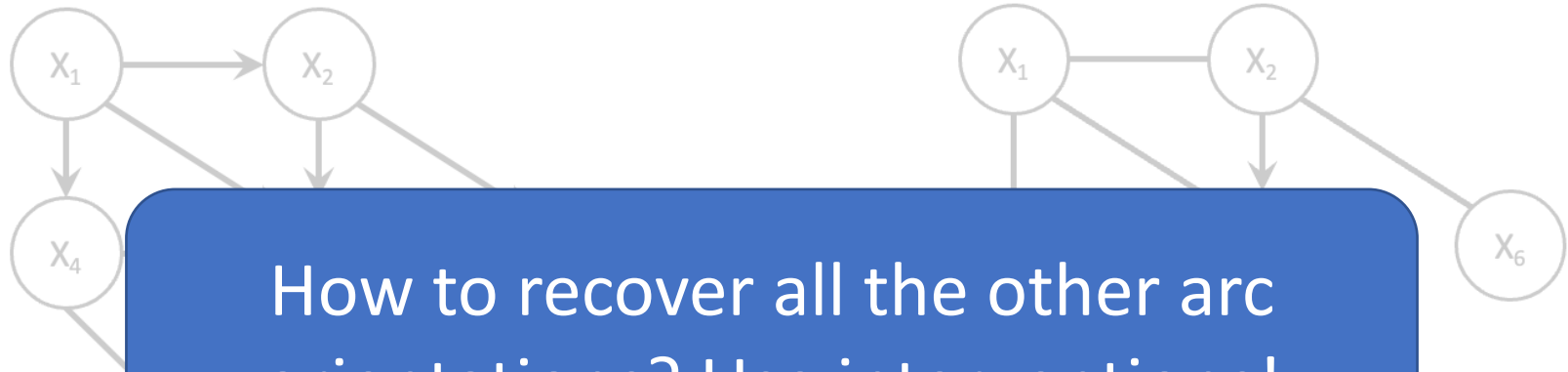


Get samples

- Recover skeleton
- Orient *some* edges

	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$
Sample 1	0.22	0.04	0.84	0.48	0.98	0.82
Sample 2	0.87	0.17	0.61	0.67	0.67	0.23
Sample 3	0.55	0.54	0.67	0.86	0.93	0.23
...	...	...	...	...	...	...
Sample M	0.12	0.95	0.79	0.47	0.05	0.92

# Structure learning (simplified)



How to recover all the other arc orientations? Use interventions!

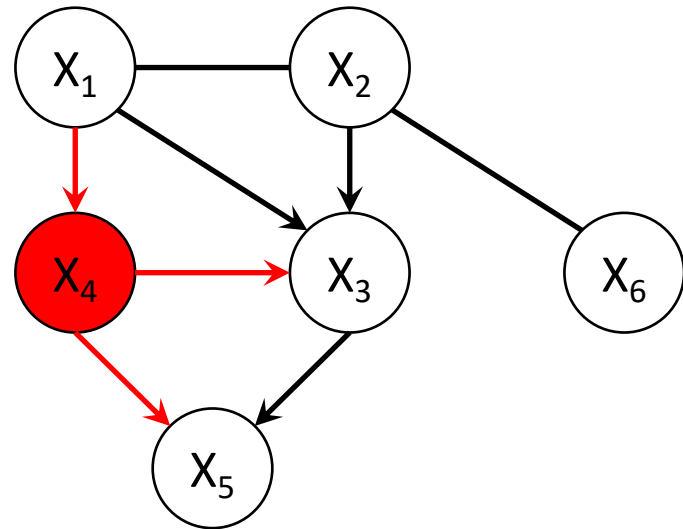
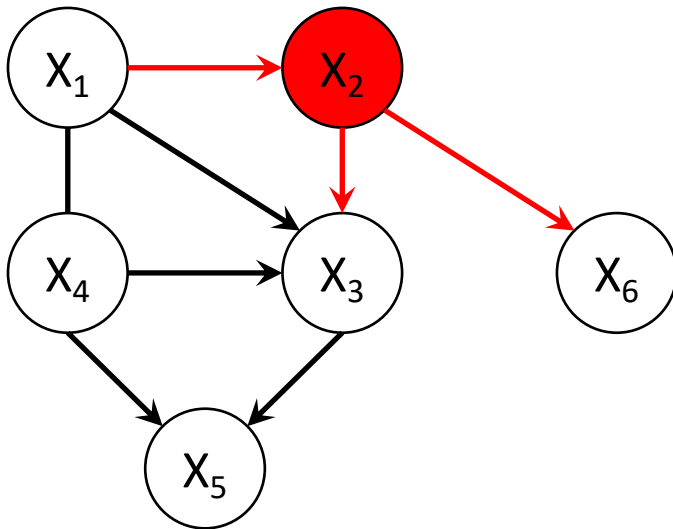
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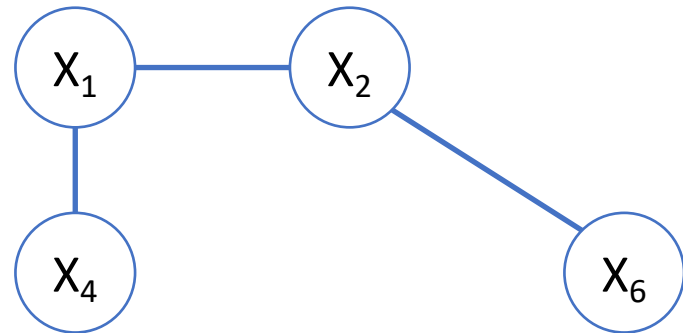
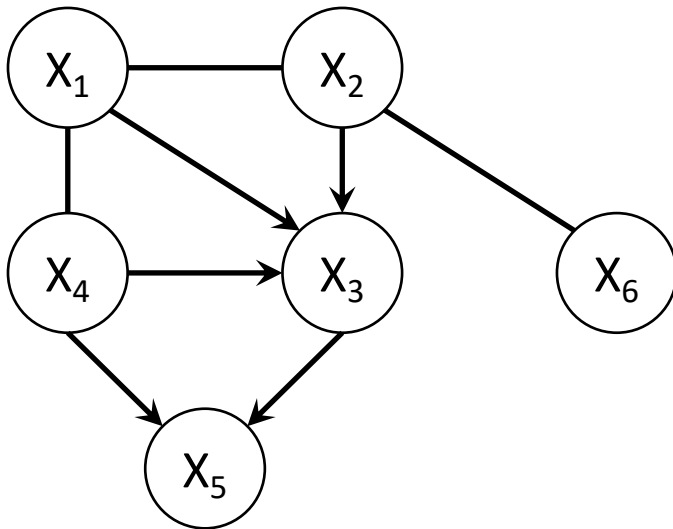
# What do interventions give us?

- When we intervene on a vertex, we recover the orientations of edges incident to the vertex



# What do interventions give us?

- When we intervene on a vertex, we recover the orientations of edges incident to the vertex



- Naïve: Compute **minimum vertex cover** on **subgraph induced by unoriented arcs**

# Meek rules [Meek 1995]

- **Sound and complete**

(with respect to arc orientations with acyclic completion)



We won't miss out on  
any information

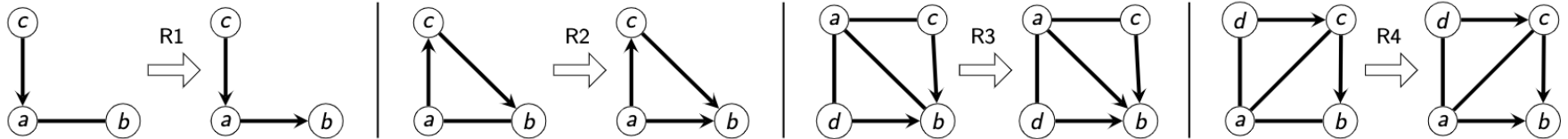
We won't wrongly  
orient arcs



# Meek rules [Meek 1995]

- **Sound and complete**

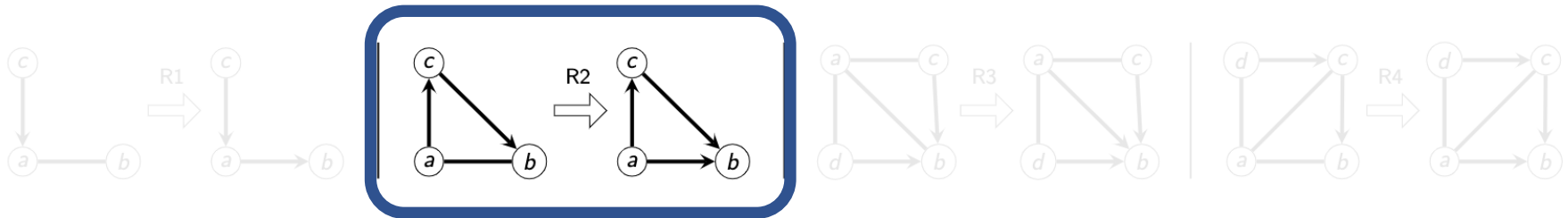
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# Meek rules [Meek 1995]

- **Sound and complete**

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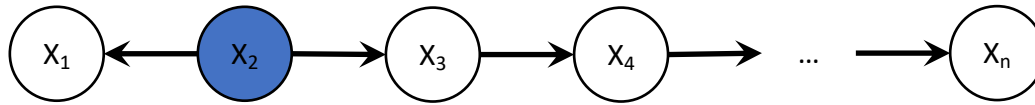


If  $b \leftarrow a$ , then cycle

- Converge in polynomial time [Wienöbst, Bannach, Liśkiewicz 2021]

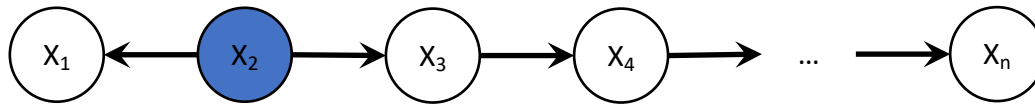
# A simple causal graph example

Hidden  
causal DAG

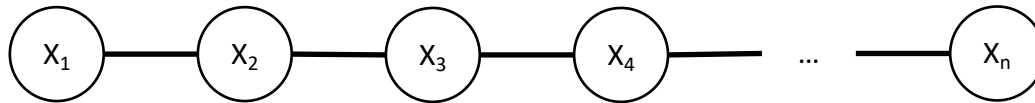


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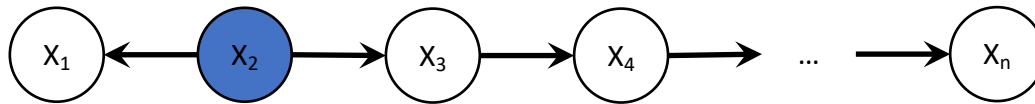


What we  
recover from  
data

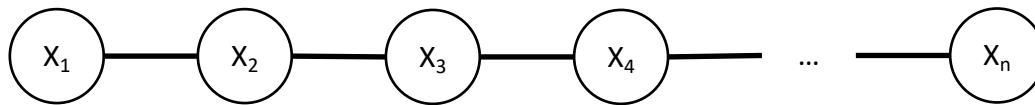


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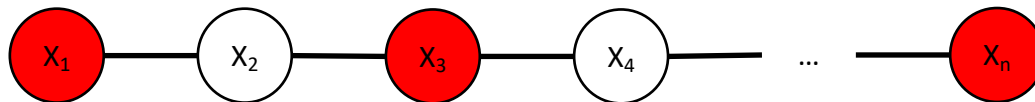
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What we recover from data

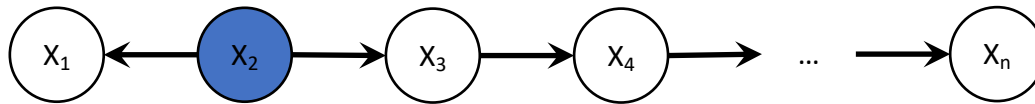


Naïve: Vertex cover

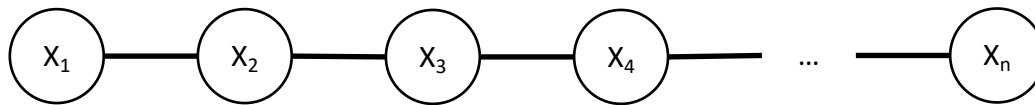


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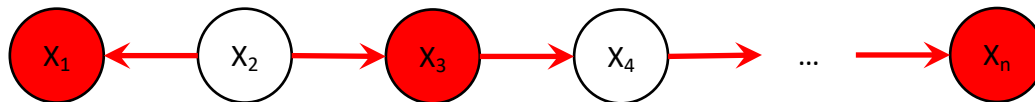
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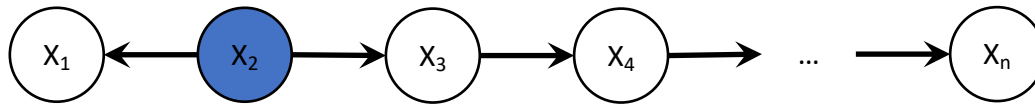


Recover incident edges

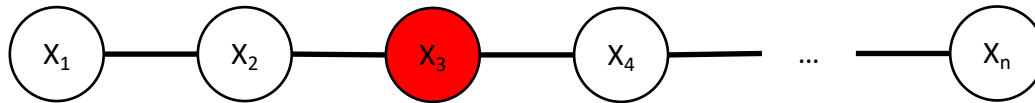
Need  $\approx \frac{n}{2}$  interventions

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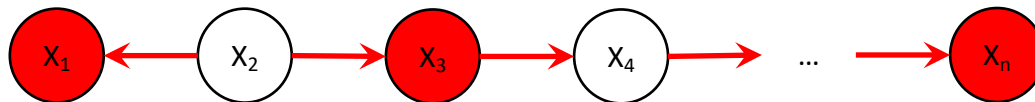
Hidden causal DAG



Suppose we intervene  $X_3$



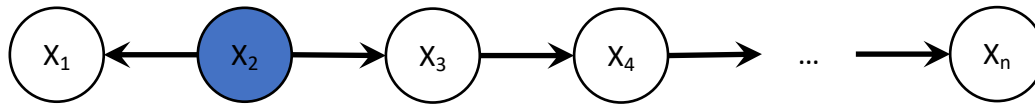
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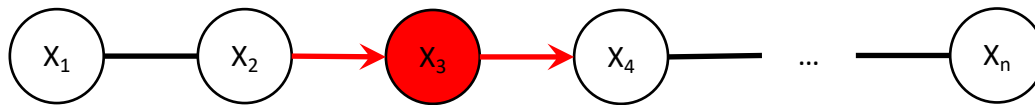
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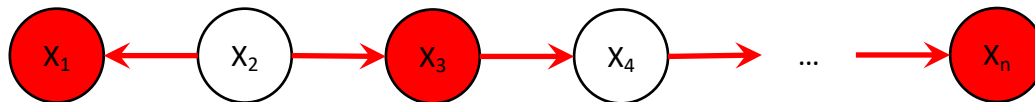


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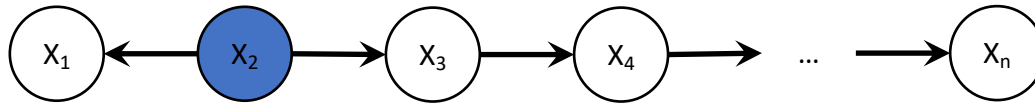


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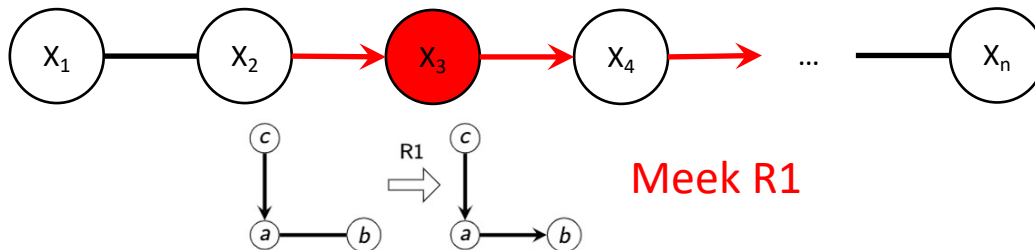


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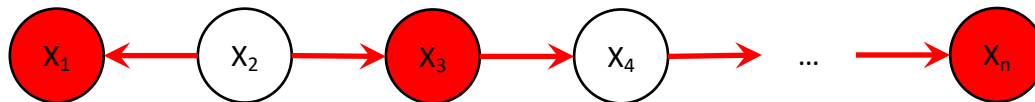


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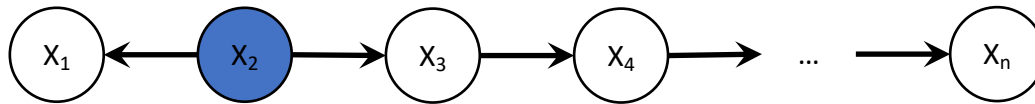
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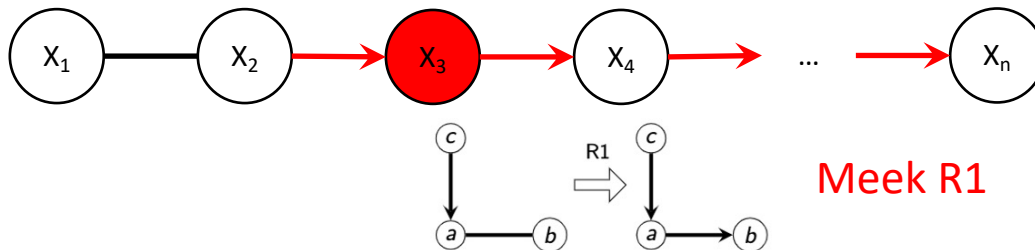
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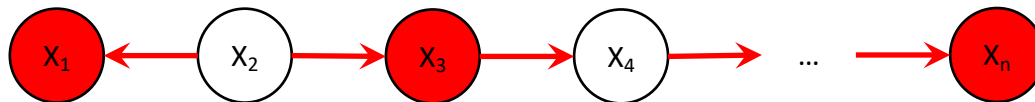


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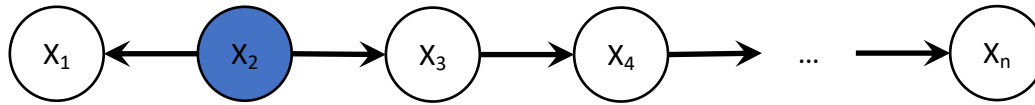


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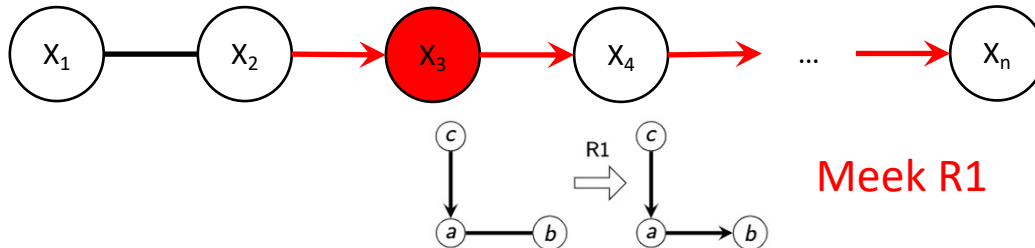
AS

Question: How many interventions do we need for this example?

Hidden causal DAG

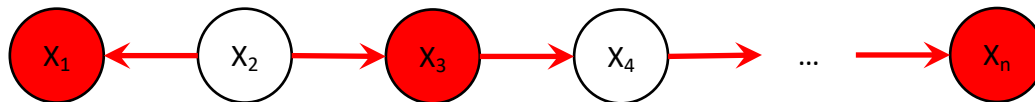


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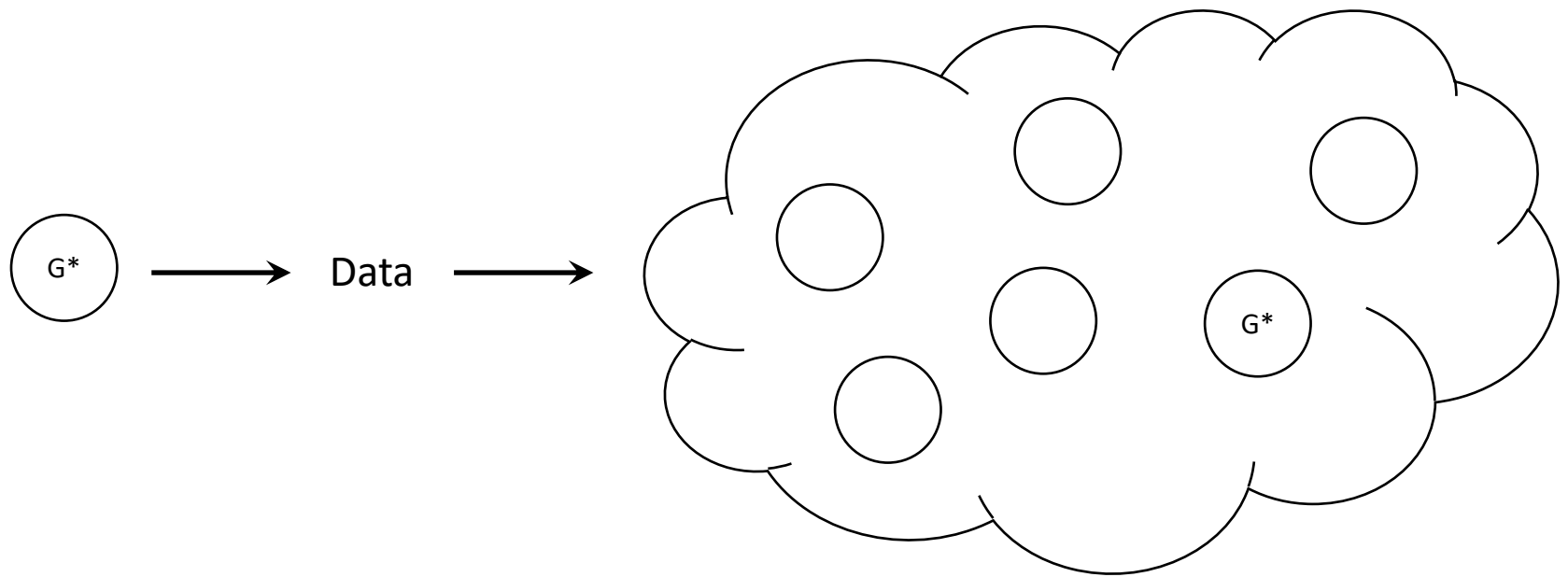
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Need  $\approx \frac{n}{2}$  interventions

# Searching using adaptive interventions

Identify  $G^*$

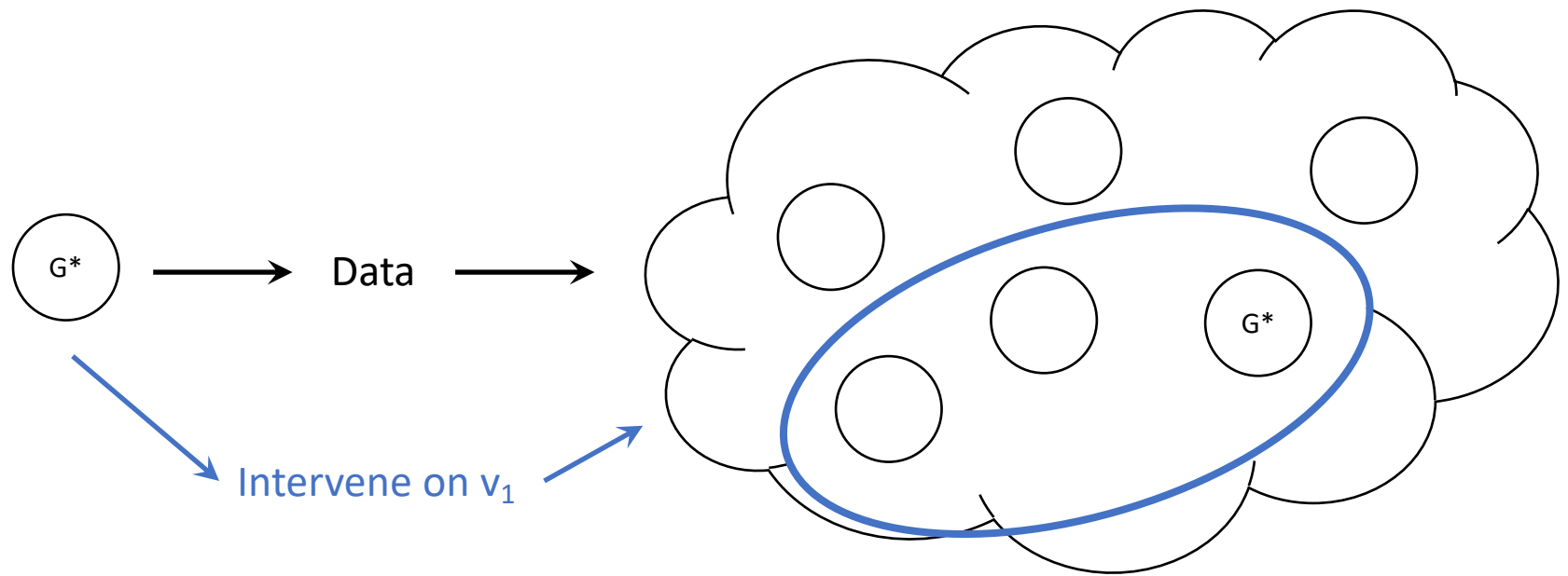


Equivalence class of causal graphs

Can be represented by a partially oriented causal graph

# Searching using adaptive interventions

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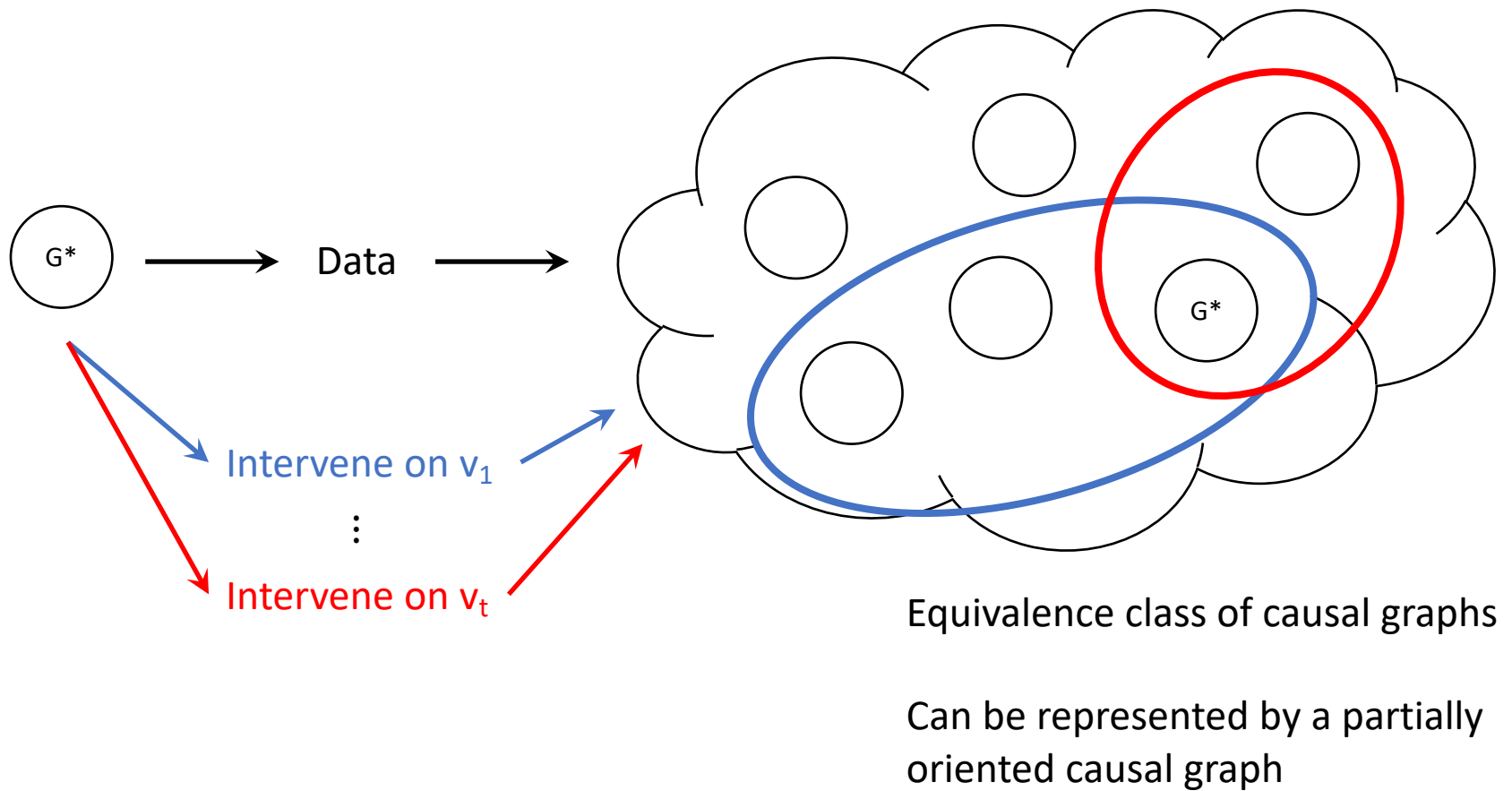


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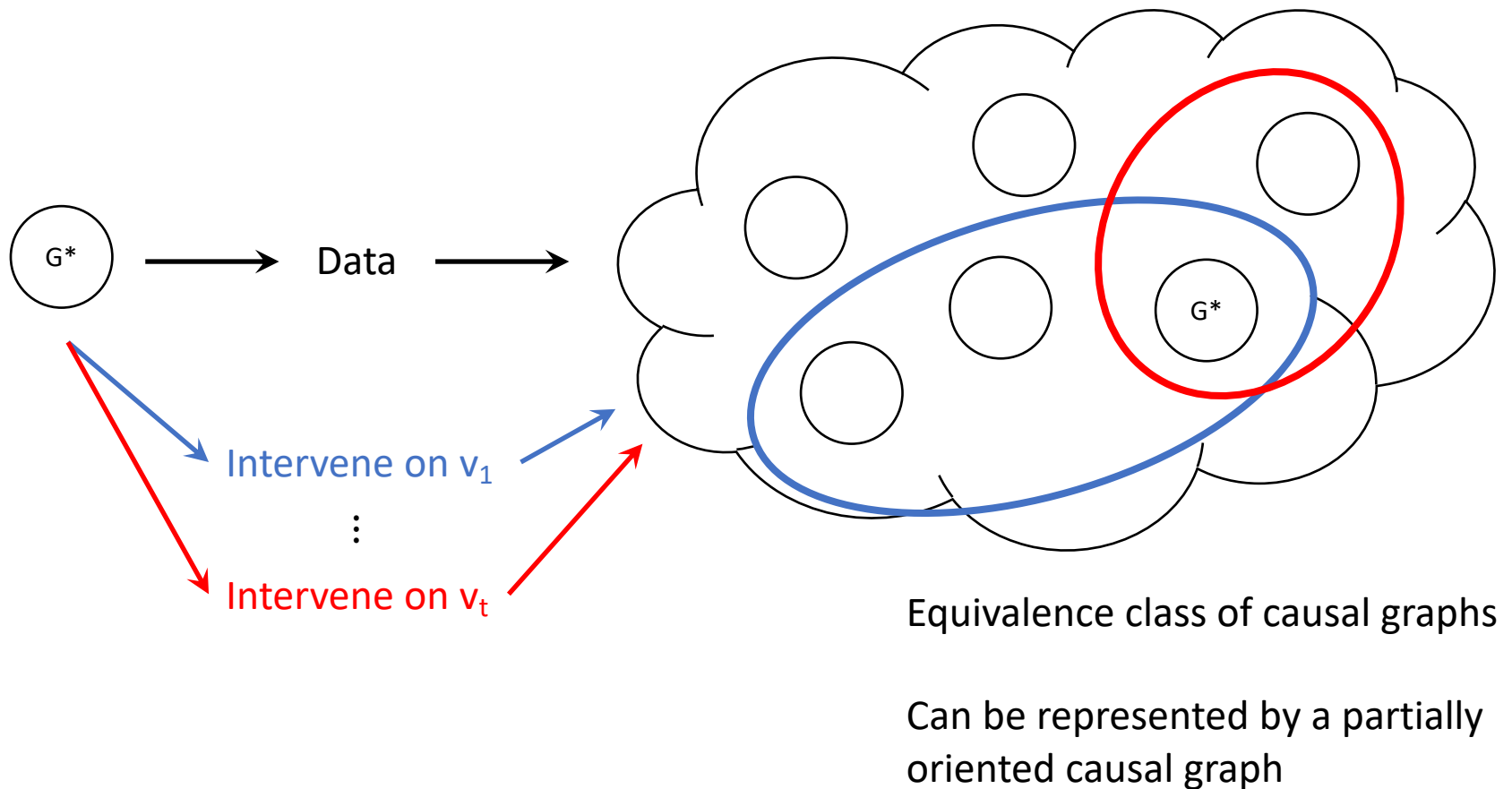
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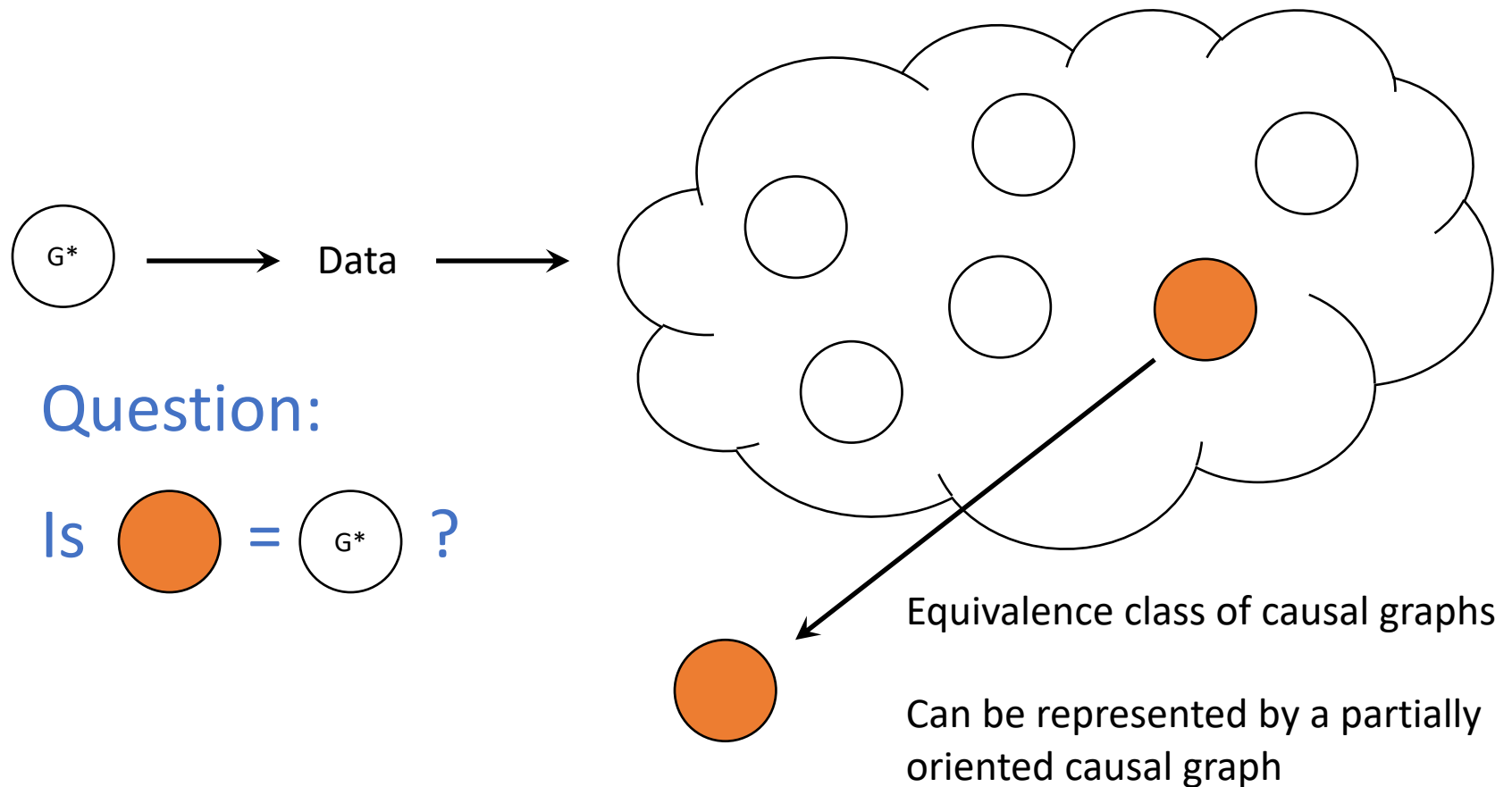


# Searching using adaptive interventions

Identify  $G^*$  using **as few interventions as possible** (minimize  $t$ )



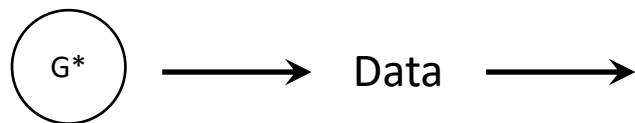
# Verification: A simpler problem





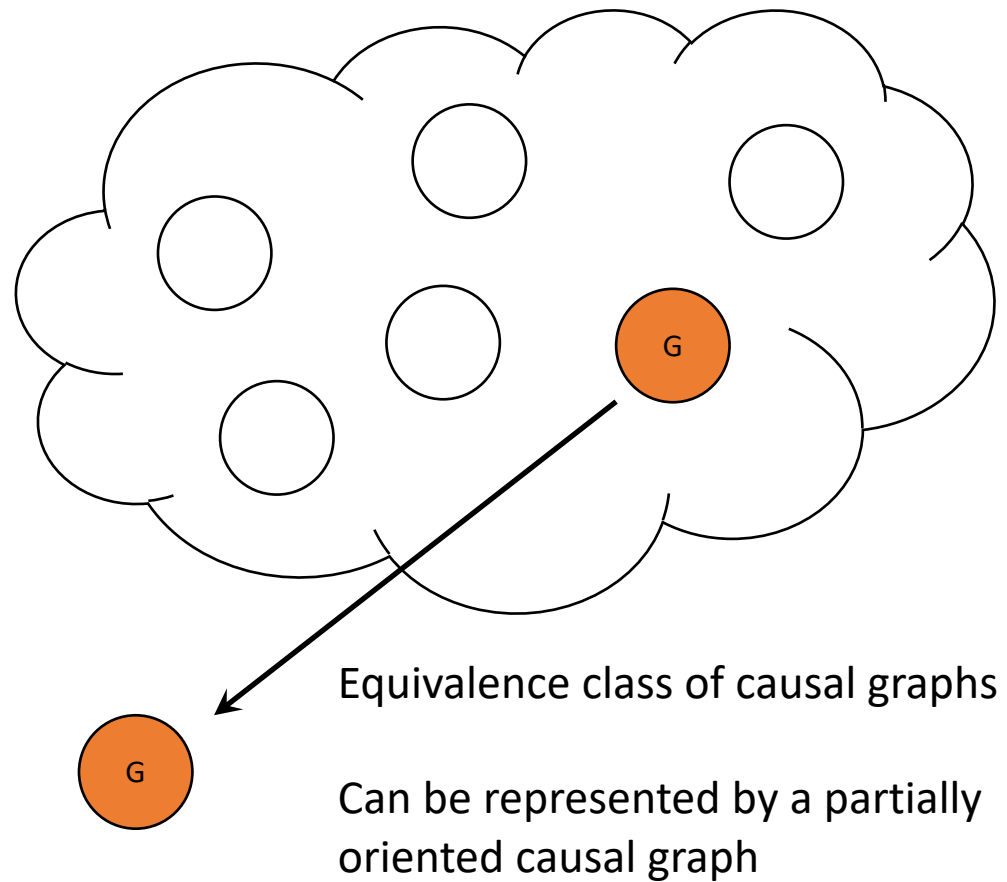
# Verification: A simpler problem

Let  $\nu(G)$  be the minimum number of interventions needed to answer this question



Question:

Is  $G = G^*$  ?



# Verification: A simpler problem

- What was known

1.  $\nu(G) \geq \left\lfloor \frac{\omega(G)}{2} \right\rfloor$  ← Maximal clique size  
[Squires, Magliacane, Greenewald, Katz, Kocaoglu, Shanmugam 2020]

2.  $\left\lfloor \frac{n-r}{2} \right\rfloor \leq \nu(G) \leq n - r$  ← Number of maximal cliques  
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- **Exact** characterization of  $\nu(G)$  for any causal DAG  $G$  via a minimum vertex cover on an induced subgraph of  $G$

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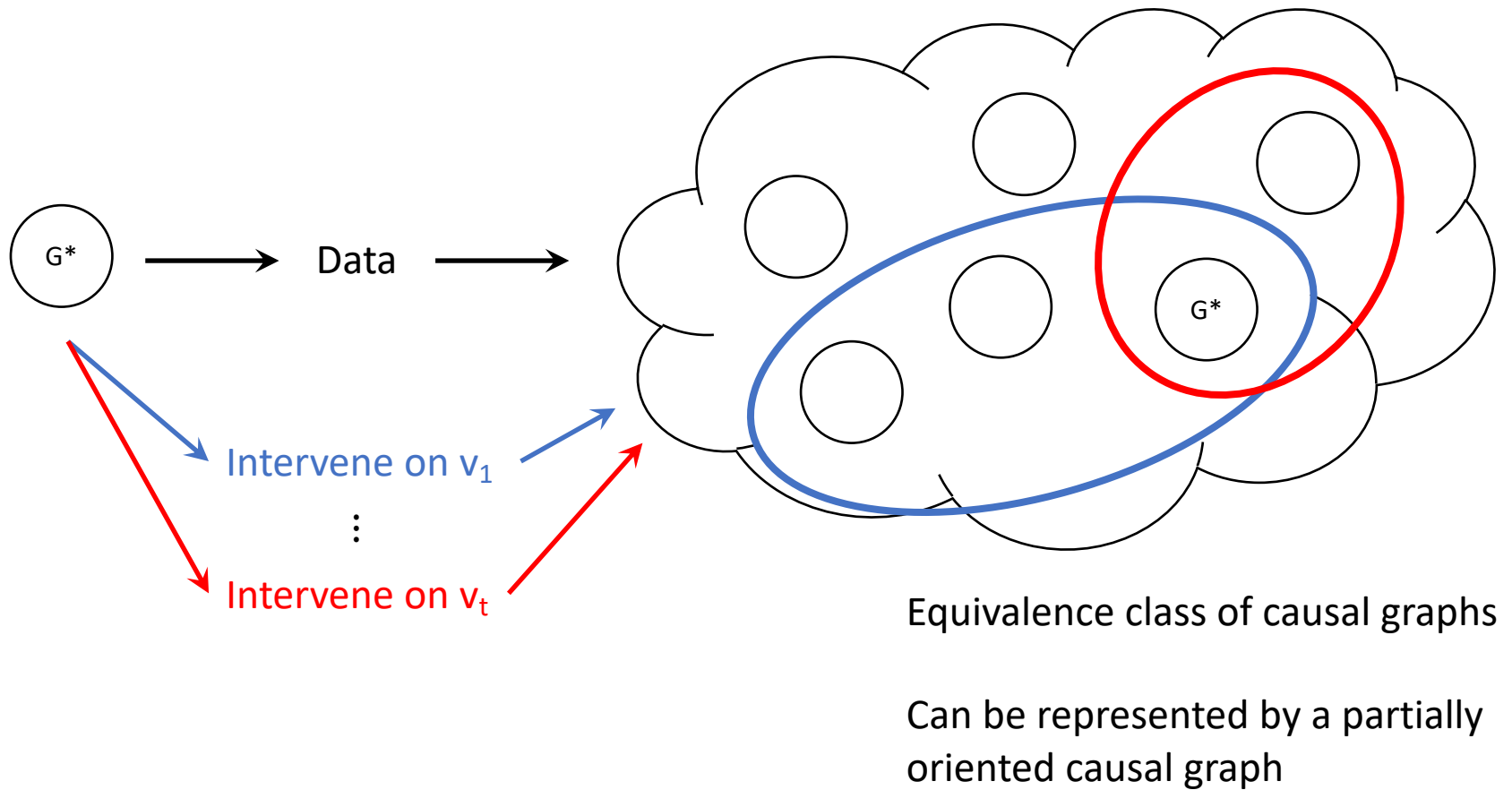
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- Proof idea: Induction on a topo ordering + Meek rules
- Efficiently computable since this subgraph is a forest

# Back to the search problem

Identify  $G^*$  using **as few interventions as possible** (minimize  $t$ )



# Two classes of interventions

- Non-adaptive

- Given equivalence class, decide on a single fixed set of interventions that recovers *any possible causal DAG*

- Need to intervene on a *G-separating system*

[Kocaoglu, Dimakis, Vishwanath 2017]



In this simplified talk, where we intervene on a single vertex per intervention, **this is just vertex cover**

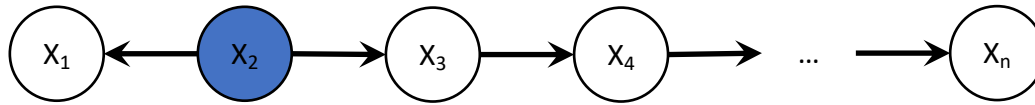
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[Kocaoglu, Dimakis, Vishwanath 2017]
- Adaptive
  - Given equivalence class,
    - Decide on first intervention
    - See outcome
    - Decide on second intervention
    - See outcome
    - ...

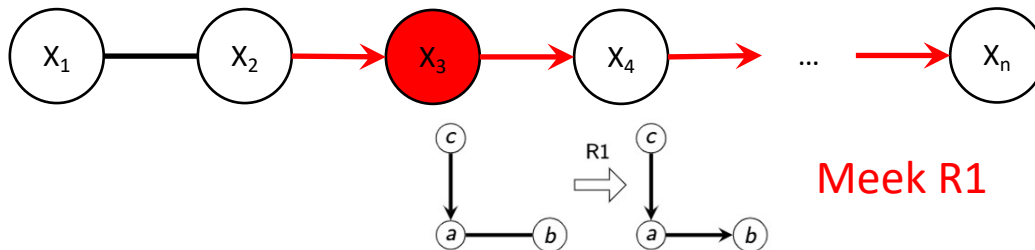


# The power of adaptivity

Hidden causal DAG

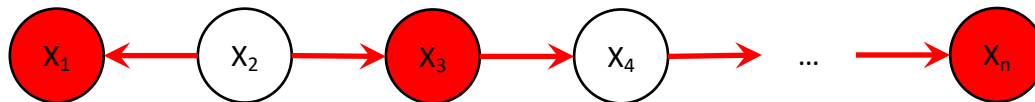


Suppose we intervene  $X_3$



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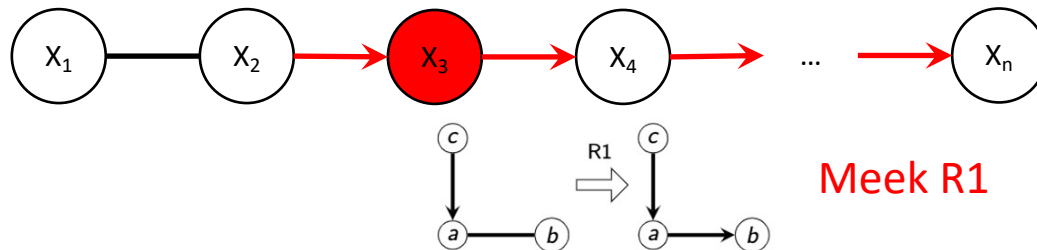
Need  $\approx \frac{n}{2}$  interventions

# The power of adaptivity

Hidden  
causal

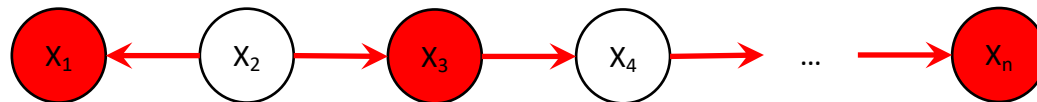
We can do something like binary search  
and only use  $\mathcal{O}(\log n)$  interventions

Suppose we  
intervene  $X_3$



$\mathcal{O}(\log n)$   
interventions  
suffice

Naïve:  
Vertex cover



Need  $\approx \frac{n}{2}$   
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# The adaptive search problem

- What we know
  - We know at least  $\nu(G^*)$  is necessary
  - Prior works only have guarantees for special classes of graphs: cliques, trees, intersection incomparable, etc.

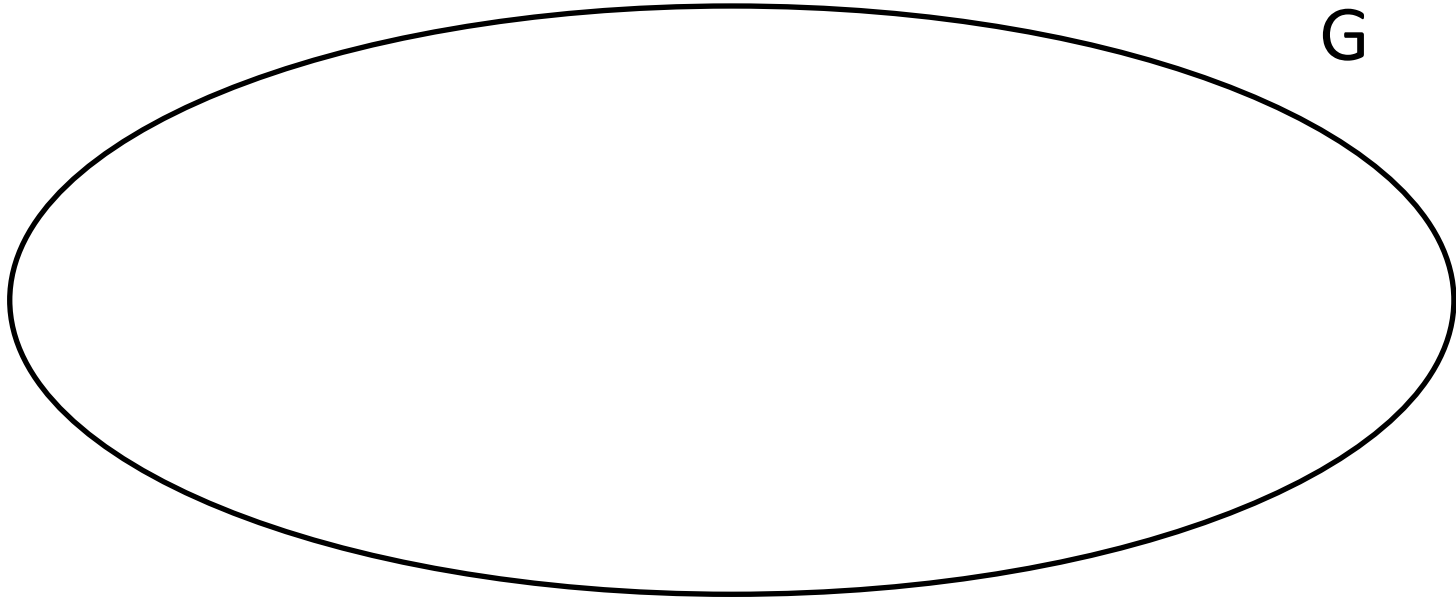
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- What we show [Choo, Shiragur, Bhattacharyya 2022]
  - Punchline:  $\mathcal{O}(\log n \cdot \nu(G^*))$  interventions suffice
  - “Search is almost as easy as verification”

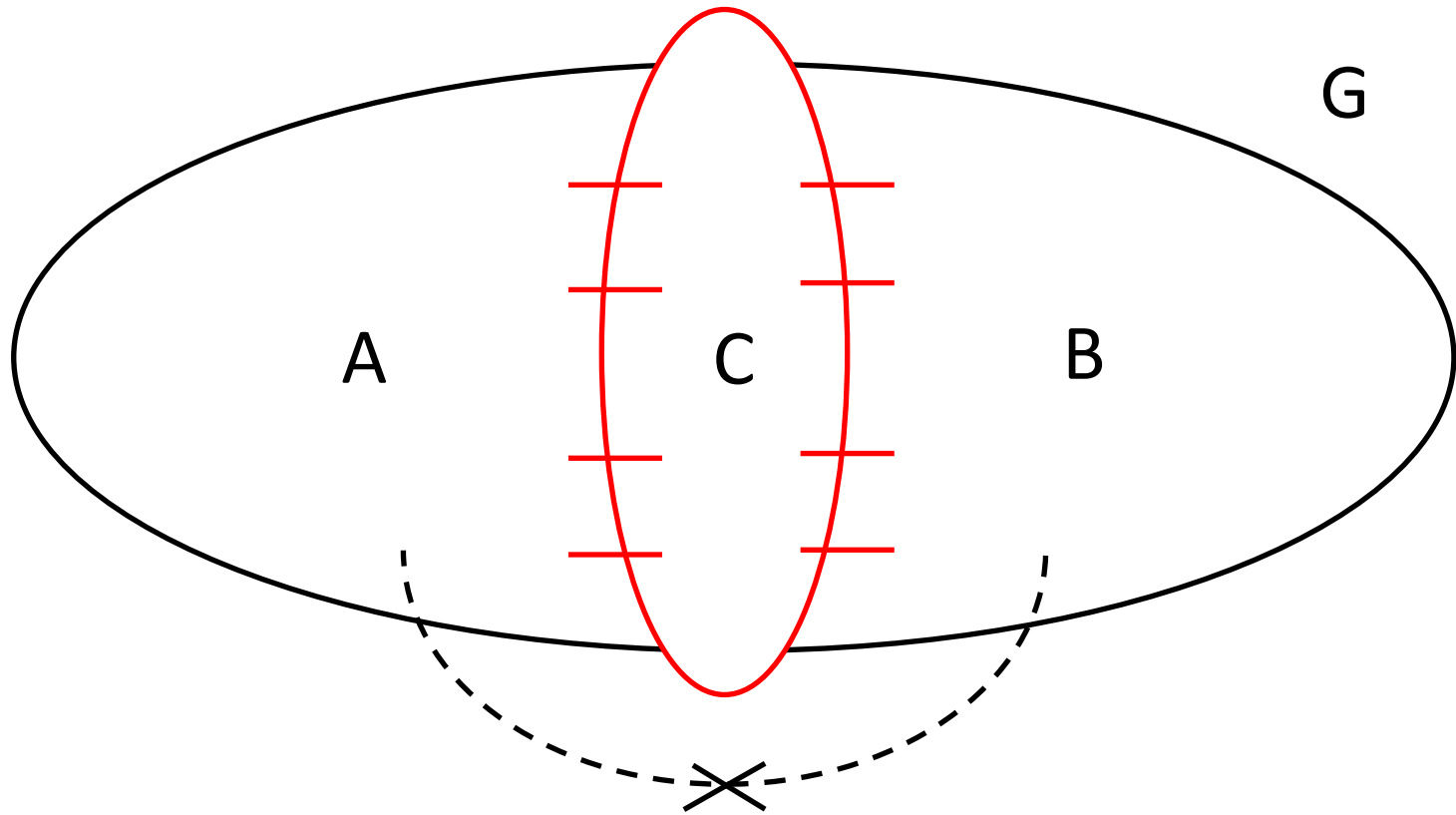
# The adaptive search problem

- What we know
  - We know at least  $v(G^*)$  is necessary
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- What we show [Choo, Shiragur, Bhattacharyya 2022]
  - Punchline:  $\mathcal{O}(\log n \cdot v(G^*))$  interventions suffice
  - “Search is almost as easy as verification”
  - Algorithm does not even know what  $v(G^*)$  is!
  - $\Omega(\log n)$  is unavoidable when causal graph is a directed path on  $n$  nodes

Key algorithmic idea: Graph separators



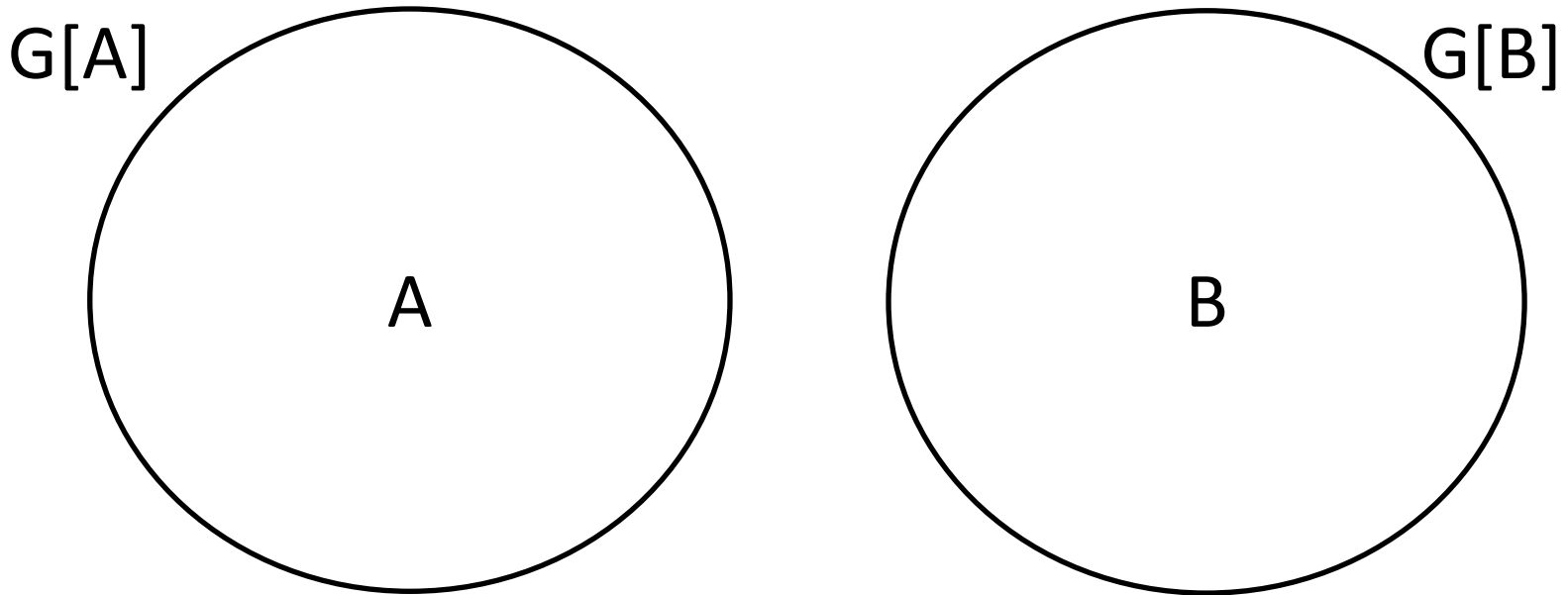
Key algorithmic idea: Graph separators



Partition vertex set  $V$  into  $A$ ,  $B$ ,  $C$ :

1.  $C$  separates  $A$  and  $B$
2.  $|A|, |B| \leq |V| / 2$

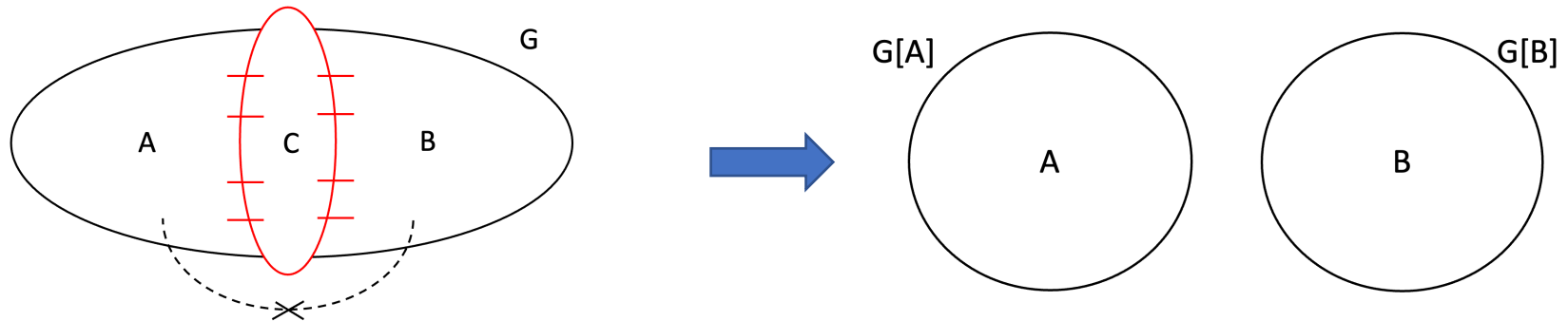
Key algorithmic idea: Graph separators



Recurse on smaller subgraphs of half the size



# Key algorithmic idea: Graph separators

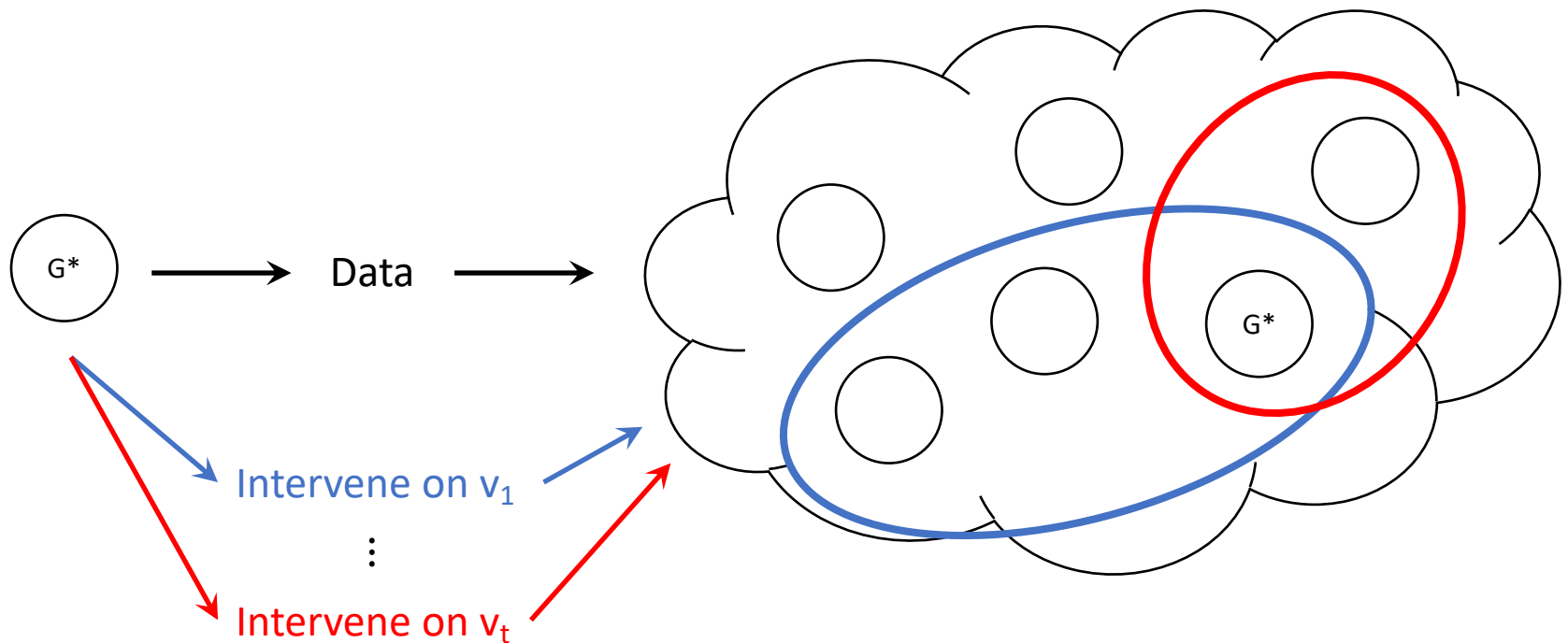


- Analysis:

- $\mathcal{O}(\log n)$  rounds  $\leftarrow$  Chordal graph separator [Gilbert, Rose, Edenbrandt 1984]
- $\mathcal{O}(v(G^*))$  per round  $\leftarrow$  We prove new lower bound on  $v(G^*)$

# Problem setup

Identify  $G^*$  using **as few interventions as possible** (minimize  $t$ )



**Verification:**  $\nu(G^*)$  = size of minimum vertex cover of covered edges

[CSB 2022]

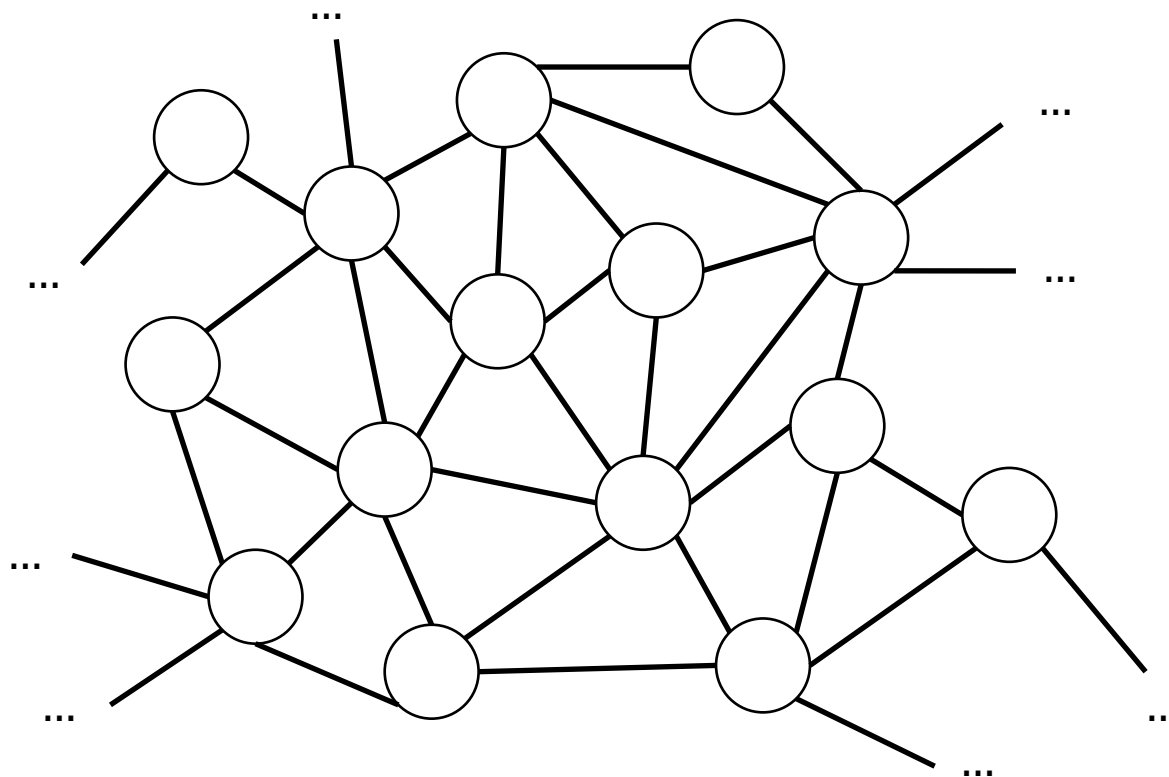
**Search:**  $\mathcal{O}(\log n \cdot \nu(G^*))$  interventions suffice

[CSB 2022]

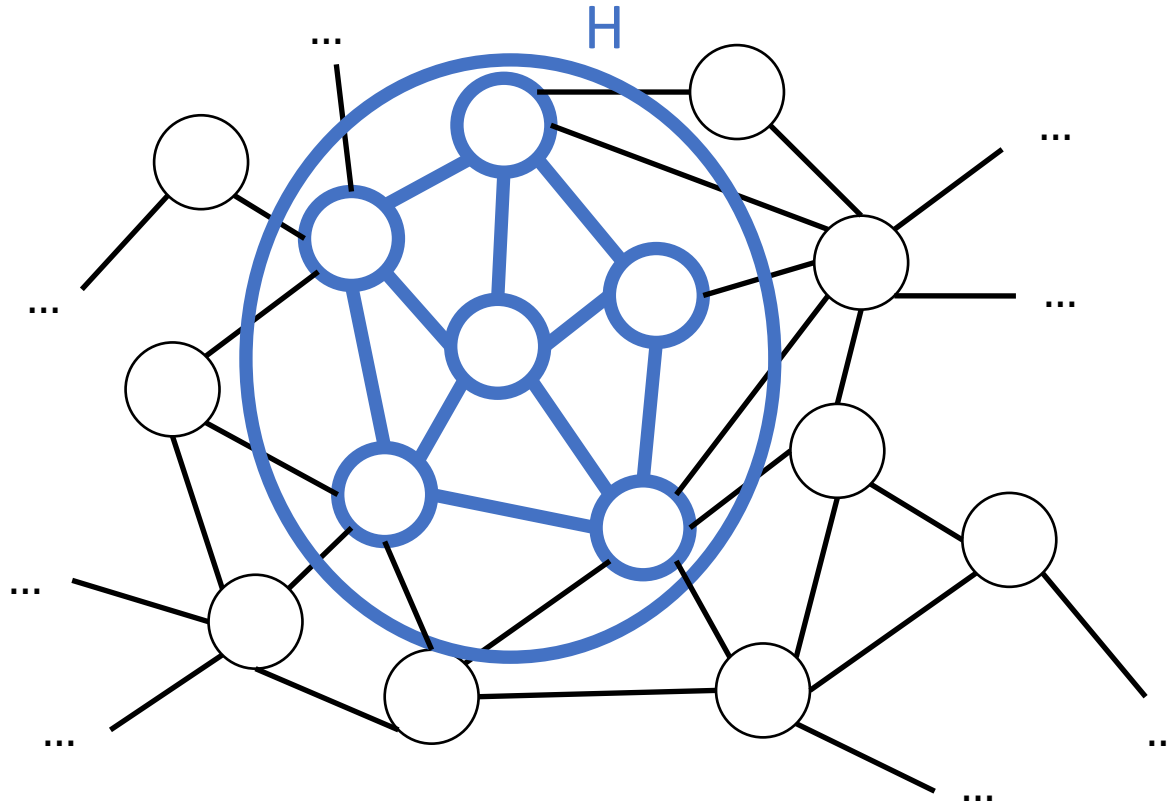
# Natural extensions and questions

- What if the causal graph is HUGE?

# What if causal graph is HUGE?



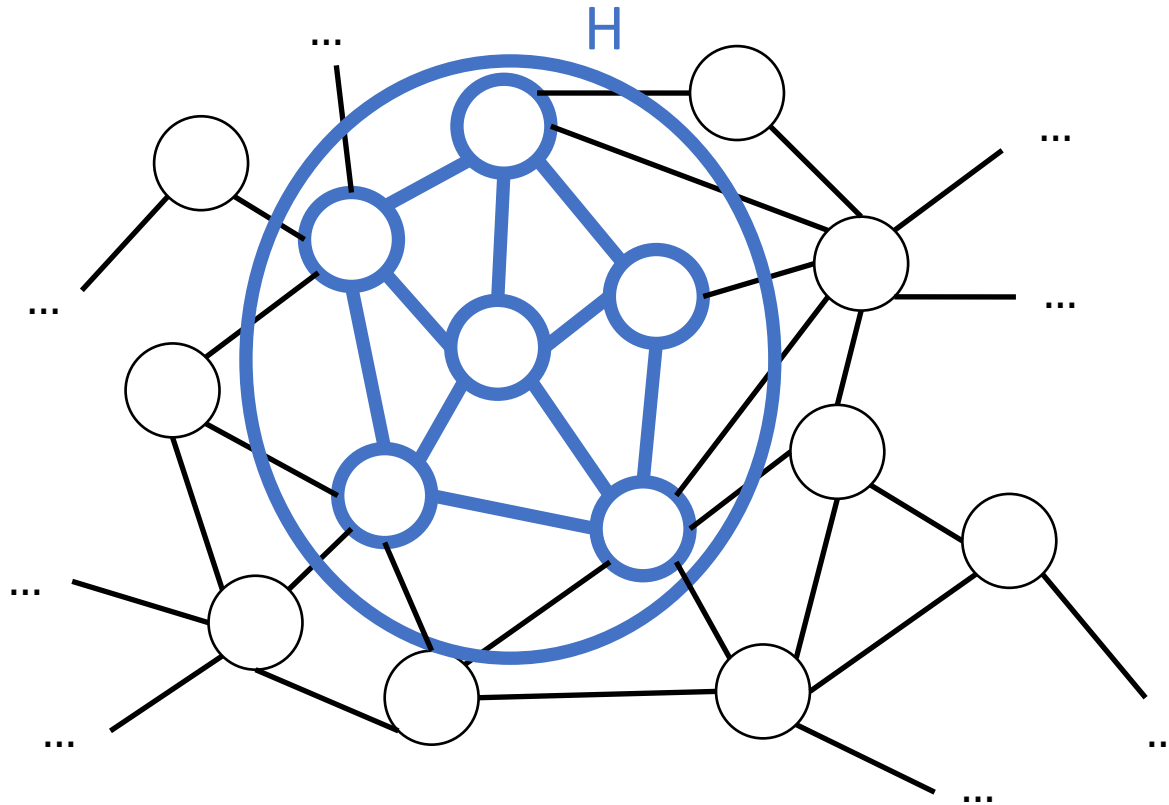
# What if causal graph is HUGE?



## **Local causal discovery:**

Only care about a small subgraph of the larger graph

# What if causal graph is HUGE?



## Local causal discovery:

Only care about a small subgraph of the larger graph

**(Informal) Verification:** Generalization of “DP on covered edge forest”.

[CS 2023]

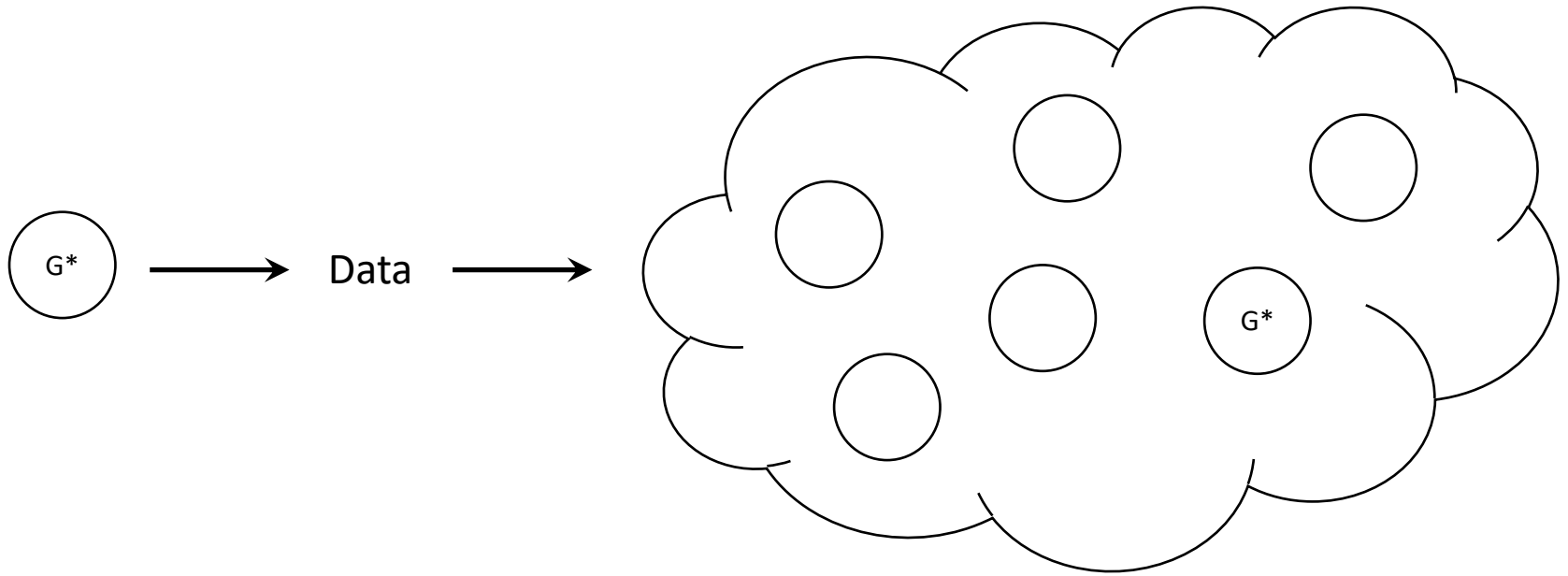
**(Informal) Search:**  $\mathcal{O}(\log |H| \cdot \nu(G^*))$  interventions suffices

[CS 2023]

# Natural extensions and questions

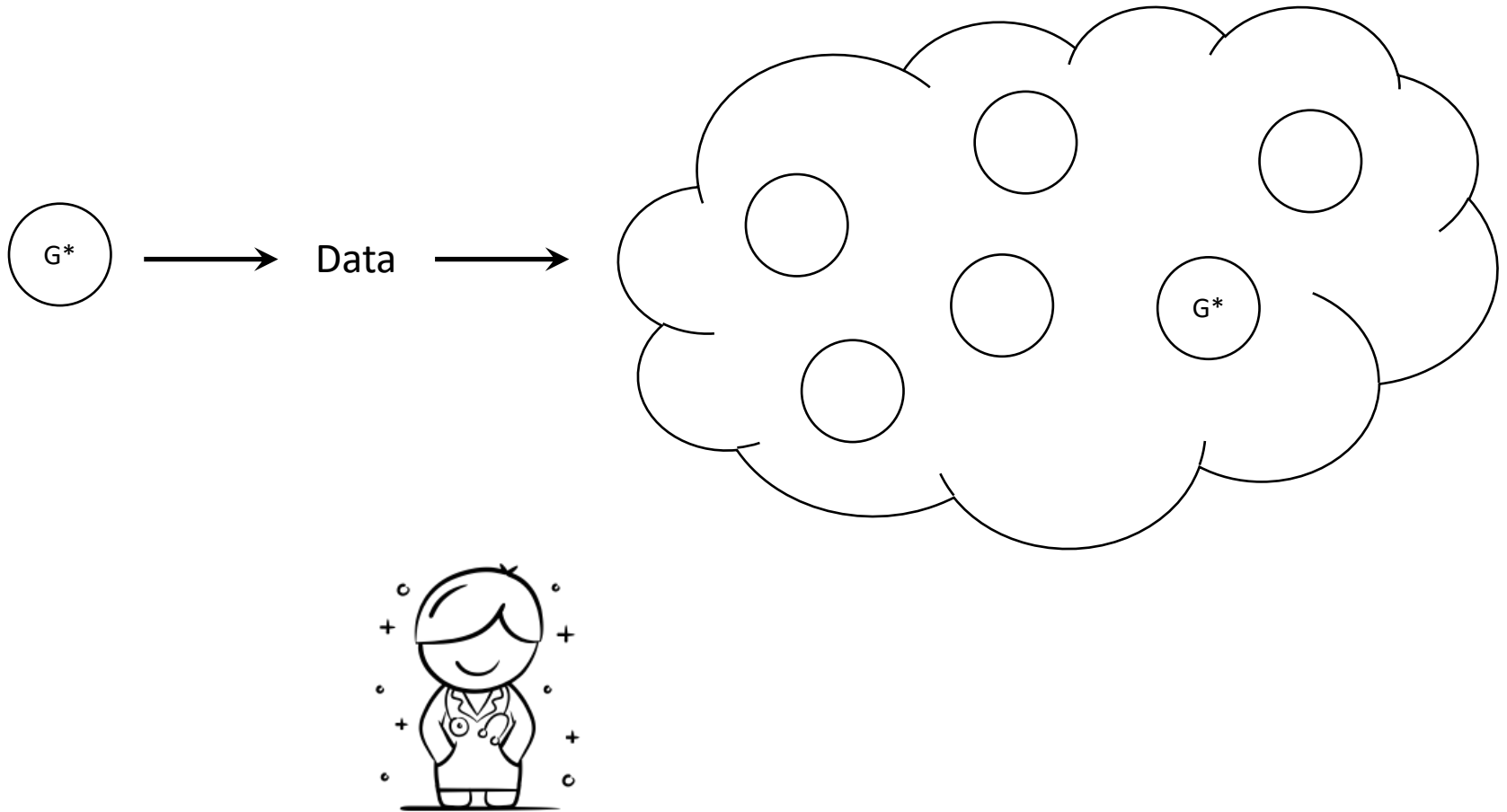
- What if the causal graph is HUGE?
- What if we consult domain experts for advice?

In many problem domains...

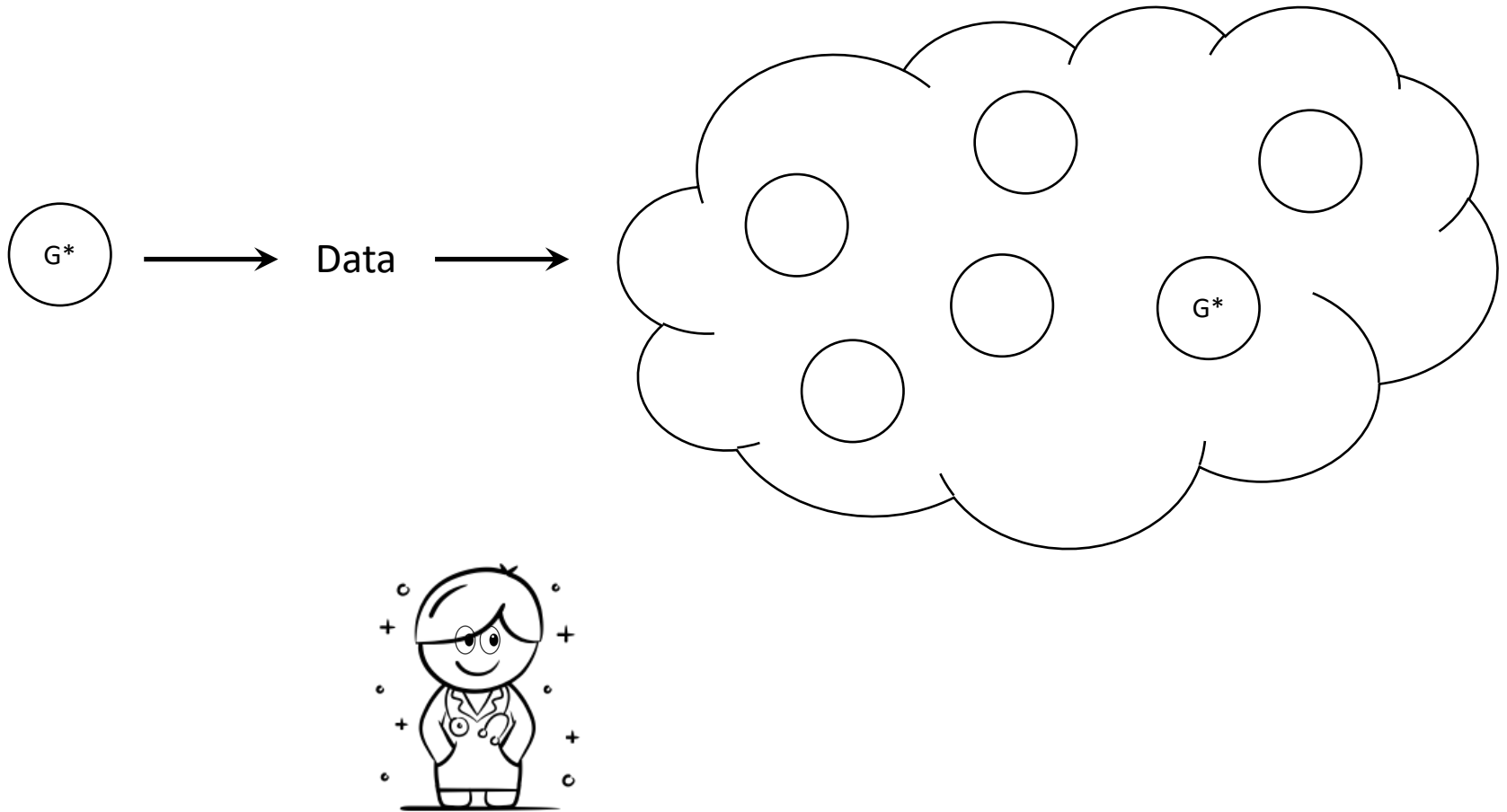




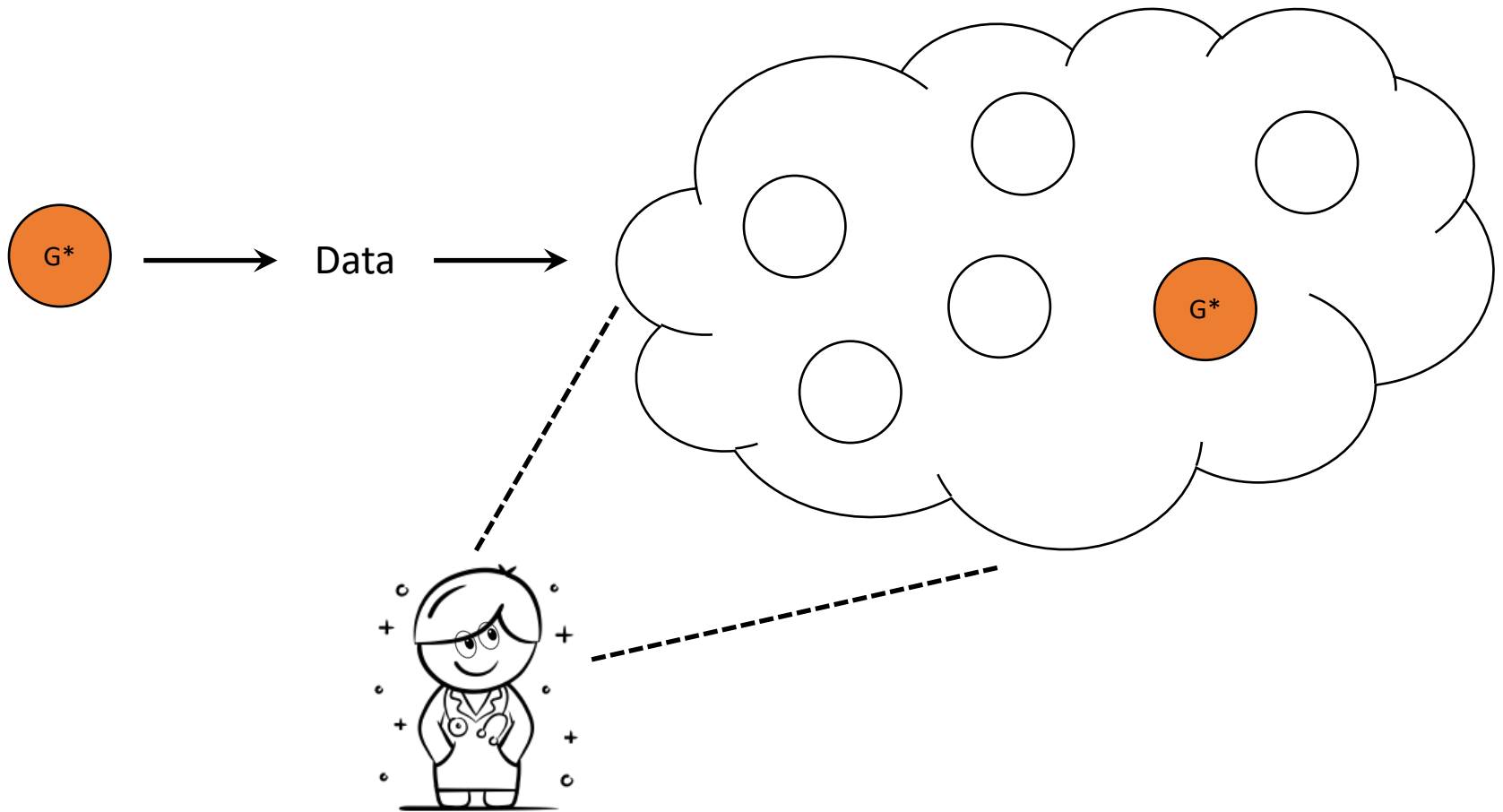
# There are domain experts!



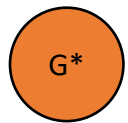
# There are domain experts!



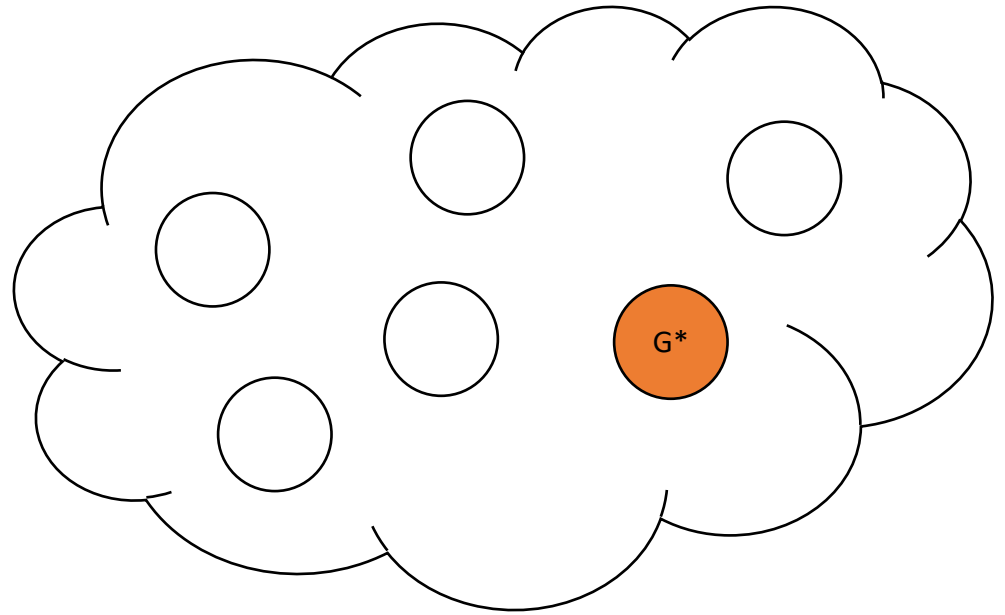
# There are domain experts!



# There are domain experts!



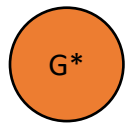
Data



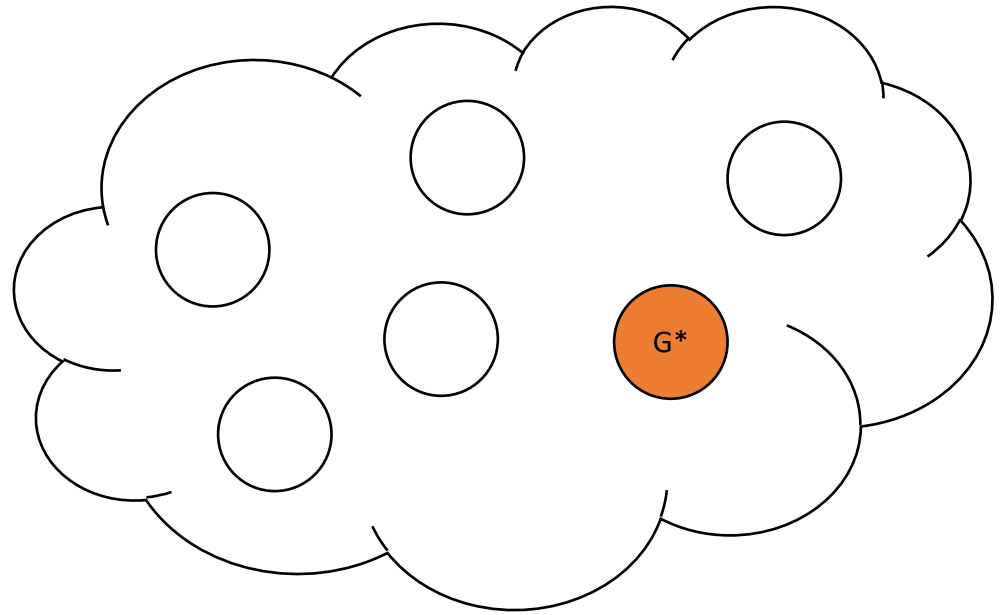
The true causal  
graph is  $G^*$  !



# There are domain experts!



→ Data →

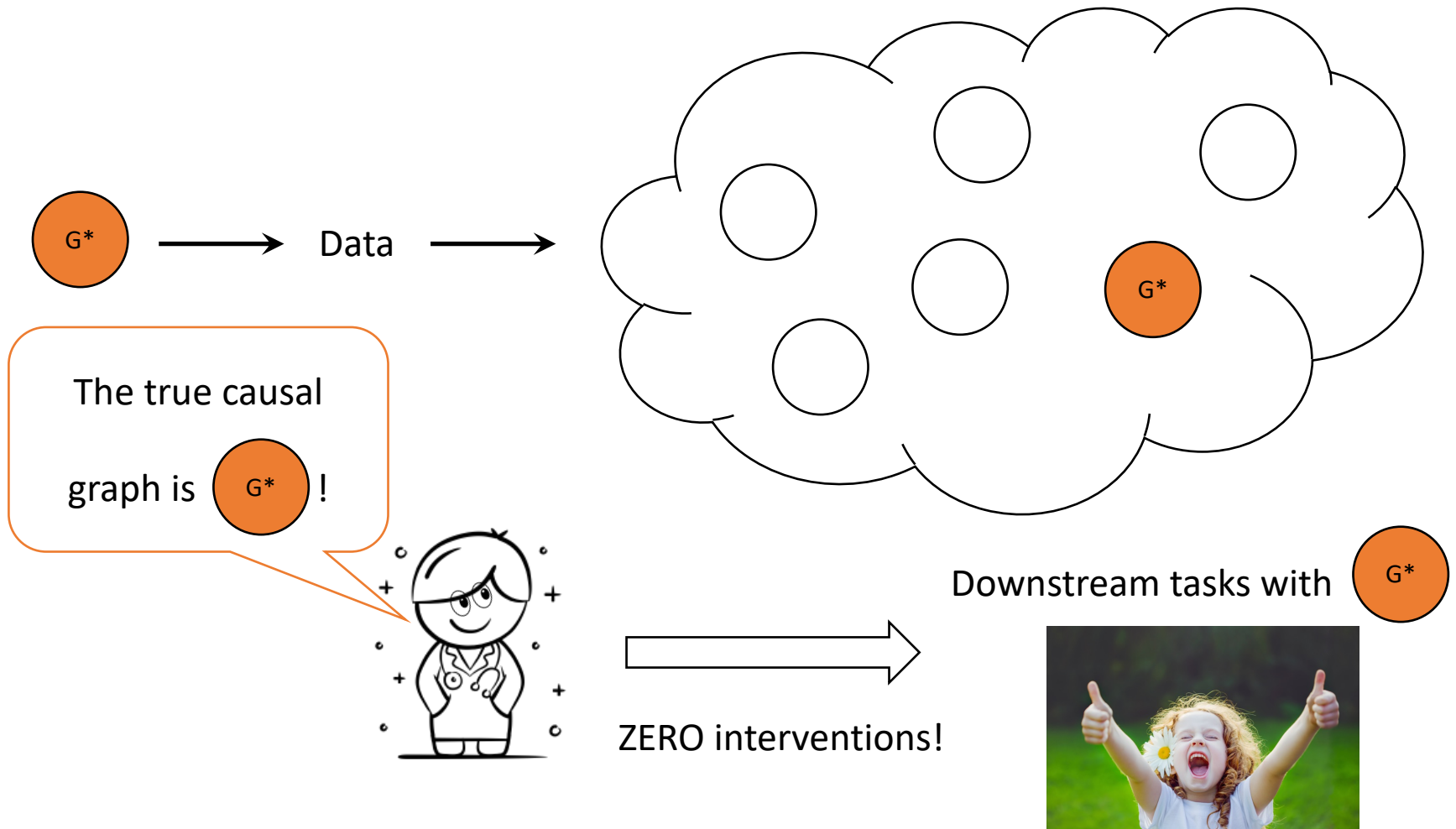


The true causal graph is  $G^*$  !

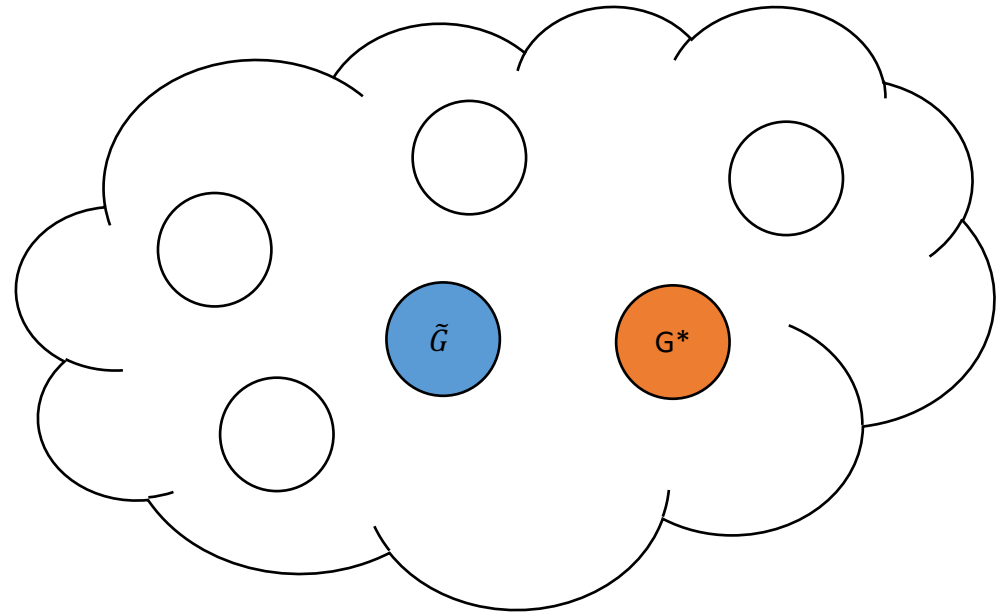
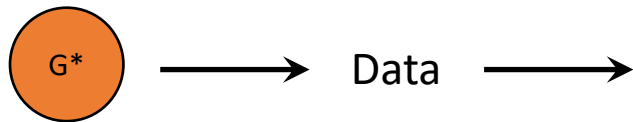


ZERO interventions!

# There are domain experts!



# But... experts can be wrong

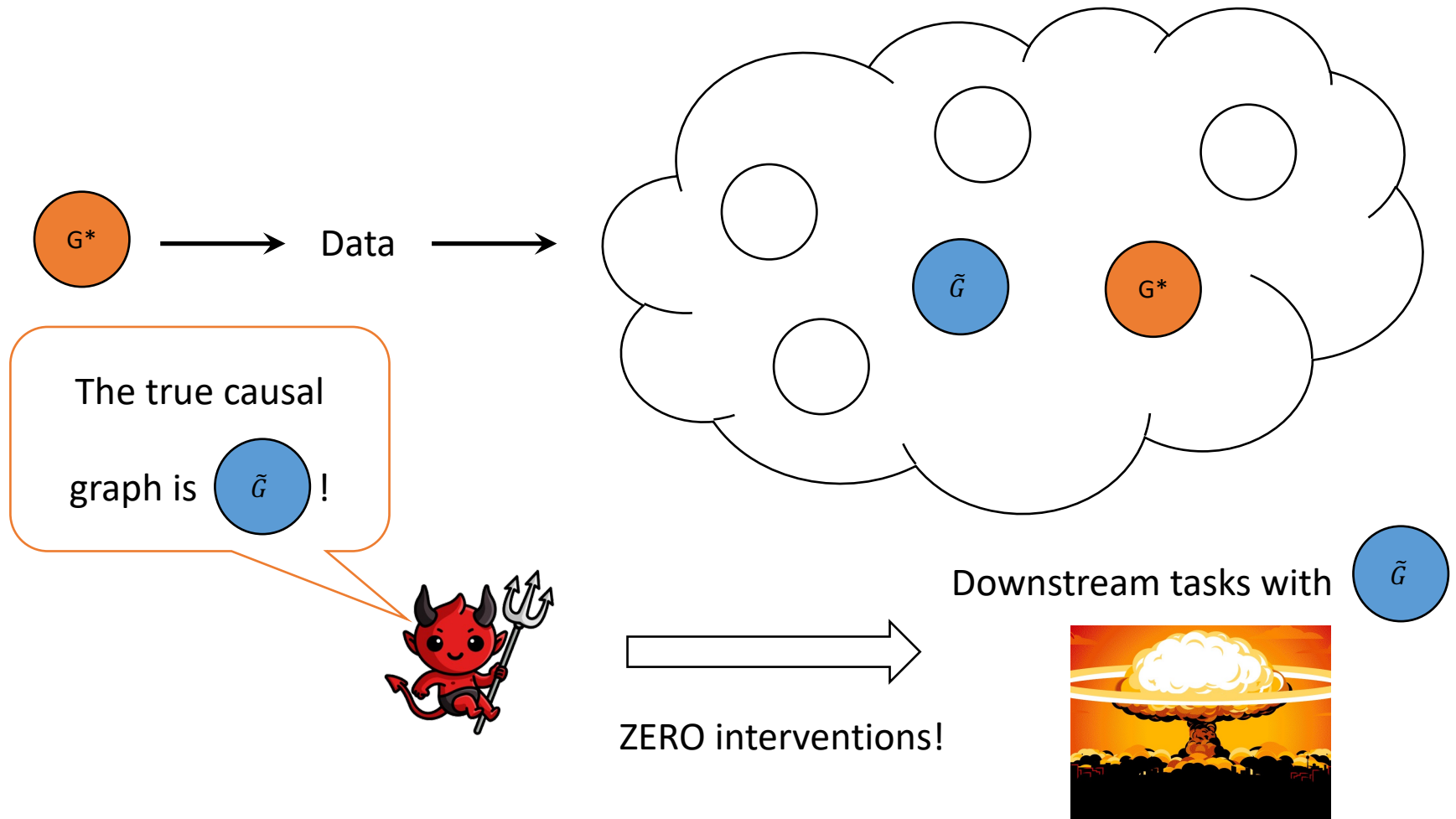


The true causal graph is  $\tilde{G}$  !



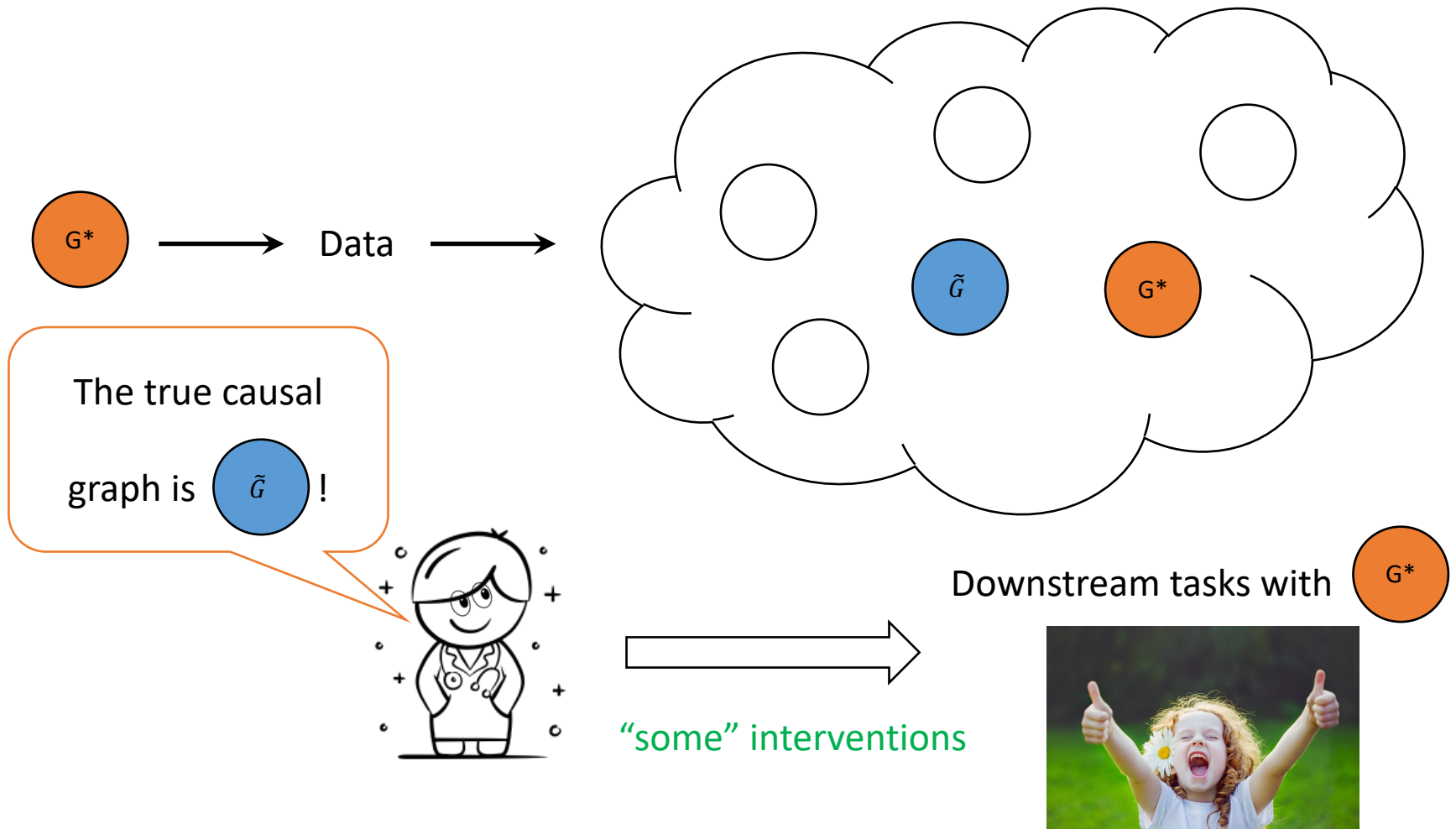
ZERO interventions!

# But... experts can be wrong

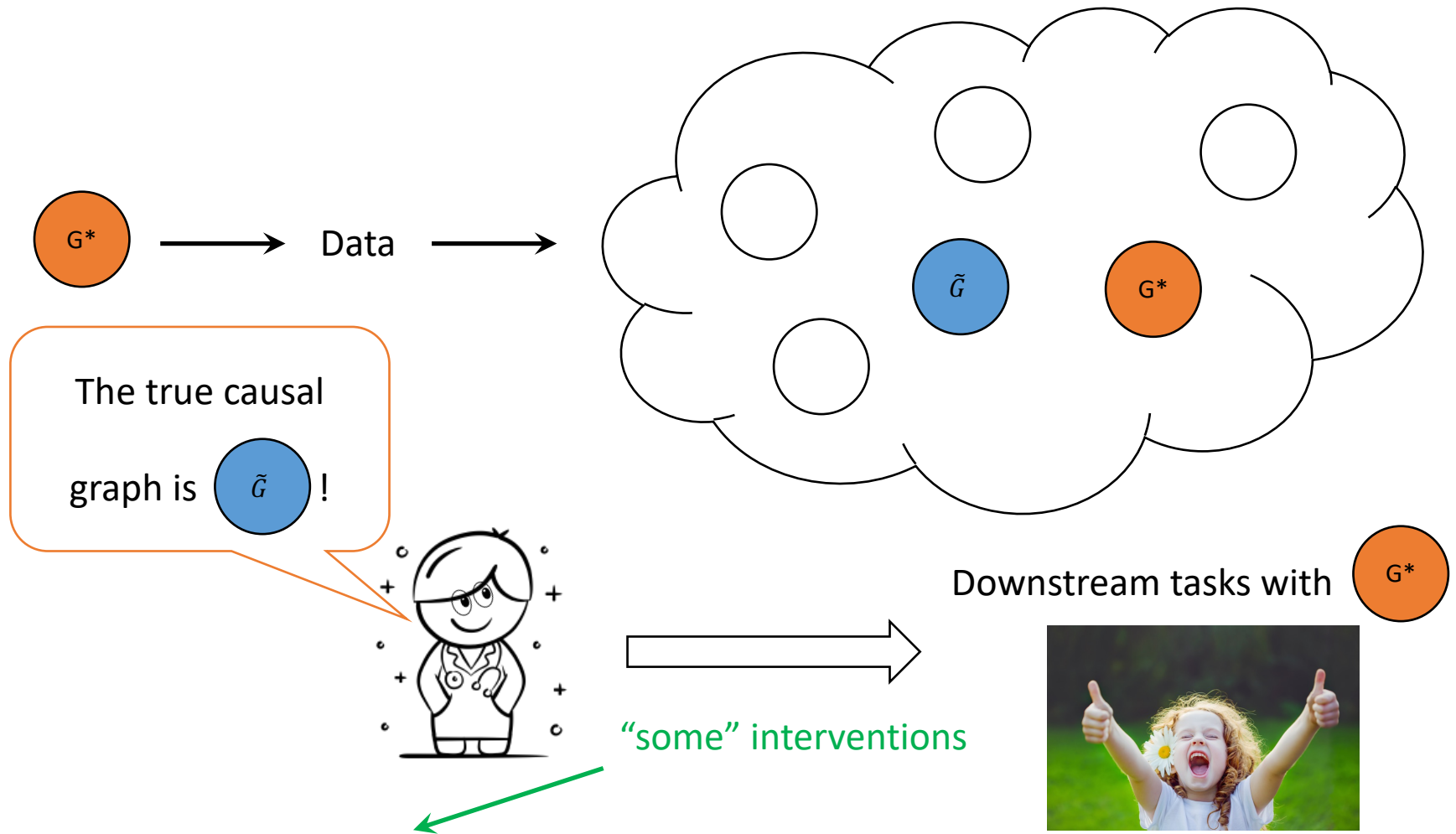




# How to use imperfect advice?



# How to use imperfect advice?



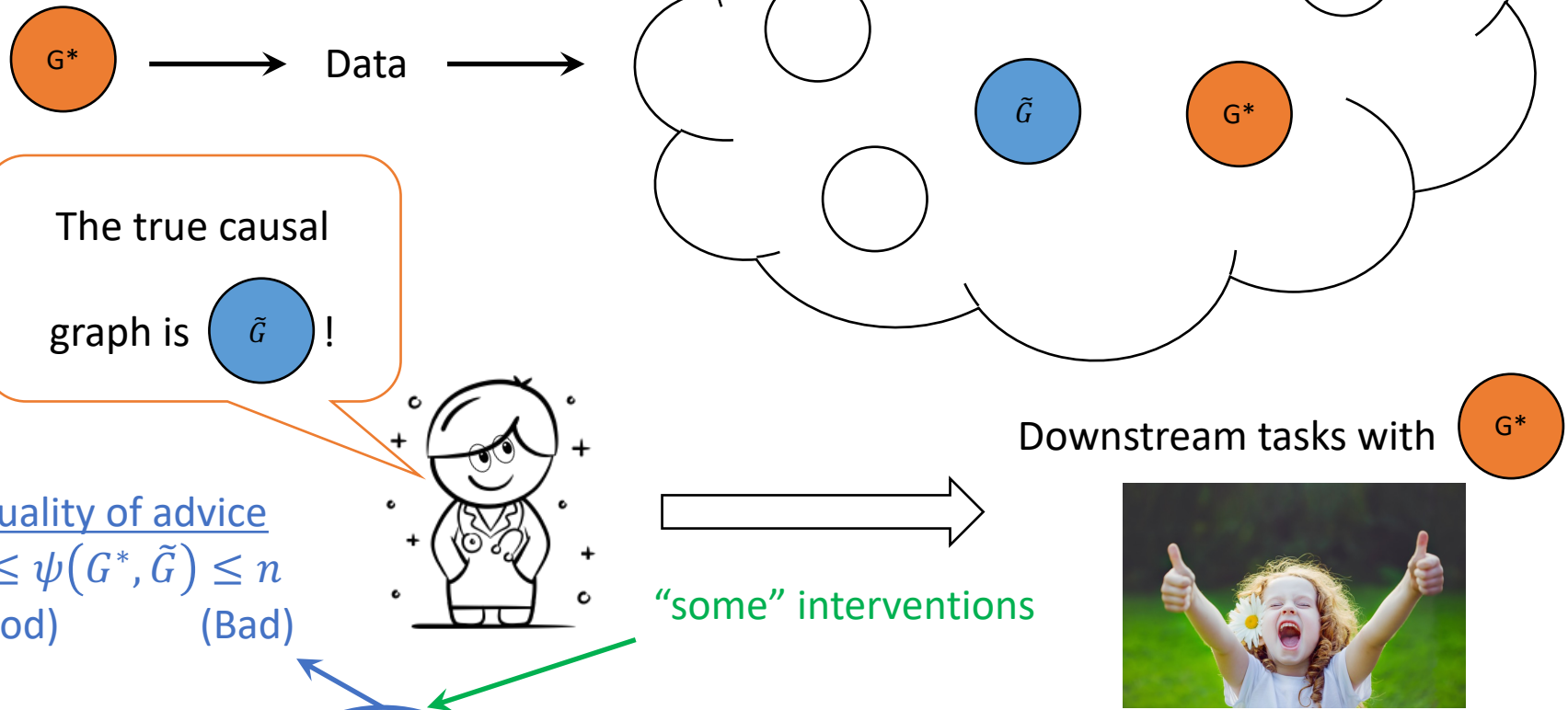
The true causal graph is  $\tilde{G}$  !

Downstream tasks with  $G^*$

“some” interventions

**Advice search:**  $\mathcal{O}(\log \psi(G^*, \tilde{G}) \cdot v(G^*))$  interventions [Choo, Gouleakis, Bhattacharyya 2023]

# How to use imperfect advice?



The true causal graph is  $\tilde{G}$  !

Quality of advice  
 $0 \leq \psi(G^*, \tilde{G}) \leq n$   
(Good) (Bad)

“some” interventions

Downstream tasks with  $G^*$



**Advice search:**  $\mathcal{O}(\log \psi(G^*, \tilde{G}) \cdot v(G^*))$  interventions [Choo, Gouleakis, Bhattacharyya 2023]

# Natural extensions and questions

- What if the causal graph is HUGE?
- What if we consult domain experts for advice?
- What if we have limited rounds of adaptivity?
- What if vertices have different interventional costs?
- What if we intervene  $>1$  vertex per intervention?
- Can we weaken/remove some causal assumptions?

# Some of our relevant papers

Choo, Shiragur, Bhattacharyya. **Verification and search algorithms for causal DAGs.** NeurIPS 2022.

Choo, Shiragur. **Subset verification and search algorithms for causal DAGs.** AISTATS 2023.

Choo, Gouleakis, Bhattacharyya. **Active causal structure learning with advice.** Submitted to ICML 2023. Under review.

Choo, Shiragur. **New metrics and search algorithms for weighted causal DAGs.** Submitted to ICML 2023. Under review.

Choo, Shiragur. **Adaptivity Complexity for Causal Graph Discovery.** Submitted to UAI 2023. Under review.