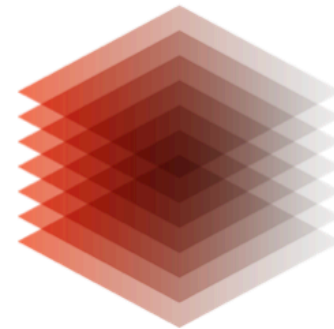


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UNIVERSITÄTSBIBLIOTHEK



TIB

Causal Relationship over Knowledge Graphs

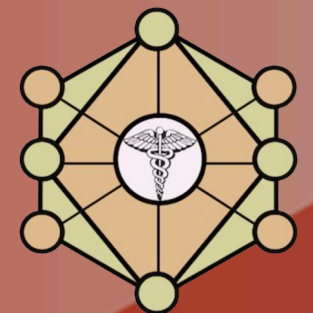
Care KG



Hao Huang
supervised by Prof. Dr. Maria-Esther Vidal

Leibniz University of Hannover, Germany
TIB Leibniz Information Centre for Science and Technology

TrustKG



funded by

Leibniz
Leibniz
Association



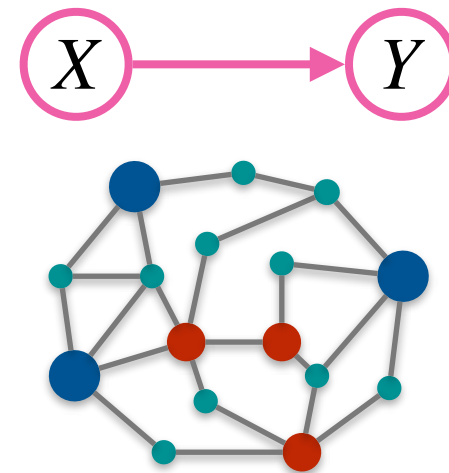
Ph.D. student at LUH
starting at 2022.01.01



Research Interests:

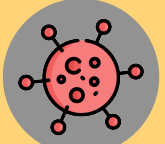


Knowledge Graphs (KGs);

Causal inference & representation over KGs;

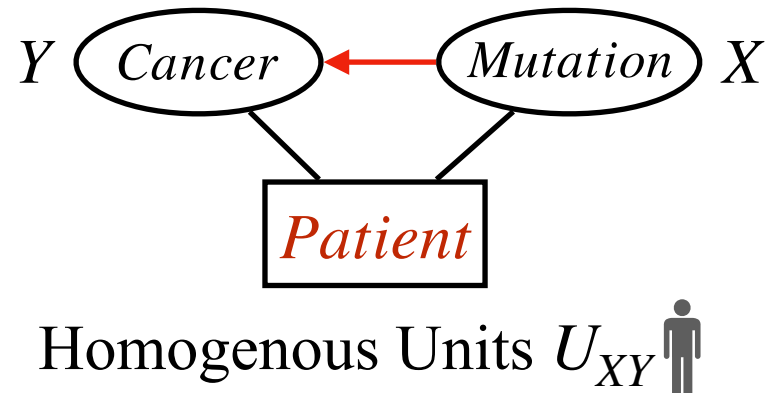


Outline

- Motivating Example
- Related Work
- Problem Statement
- CareKG-Proposed Solution
- Experimental Study
- Lessons Learned & Timeline
- Conclusions & Future Work

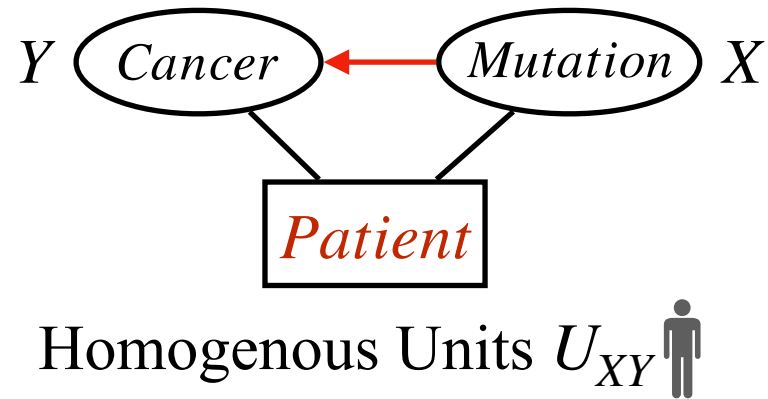
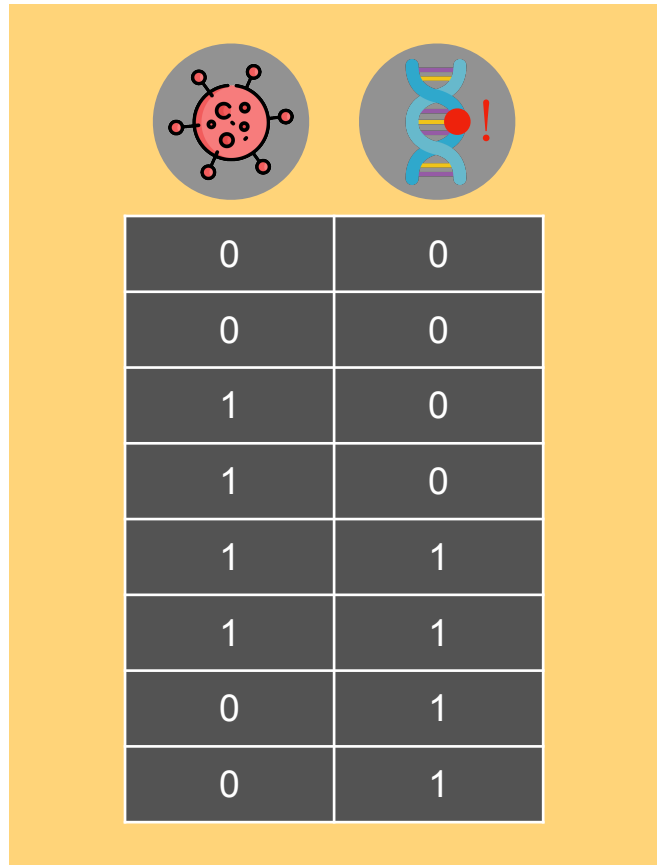
0	0
0	0
1	0
1	0
1	1
1	1
0	1
0	1



Contingency Matrix

	Cancer	No Cancer
Mutation	2	2
No Mutation	2	2

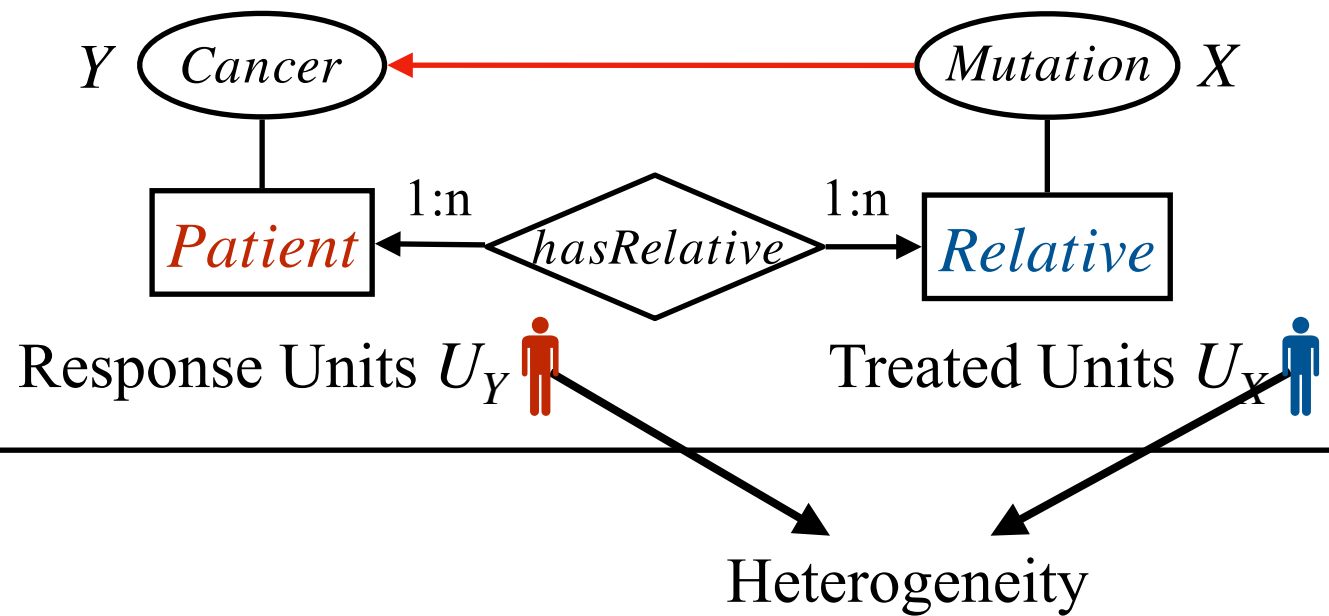
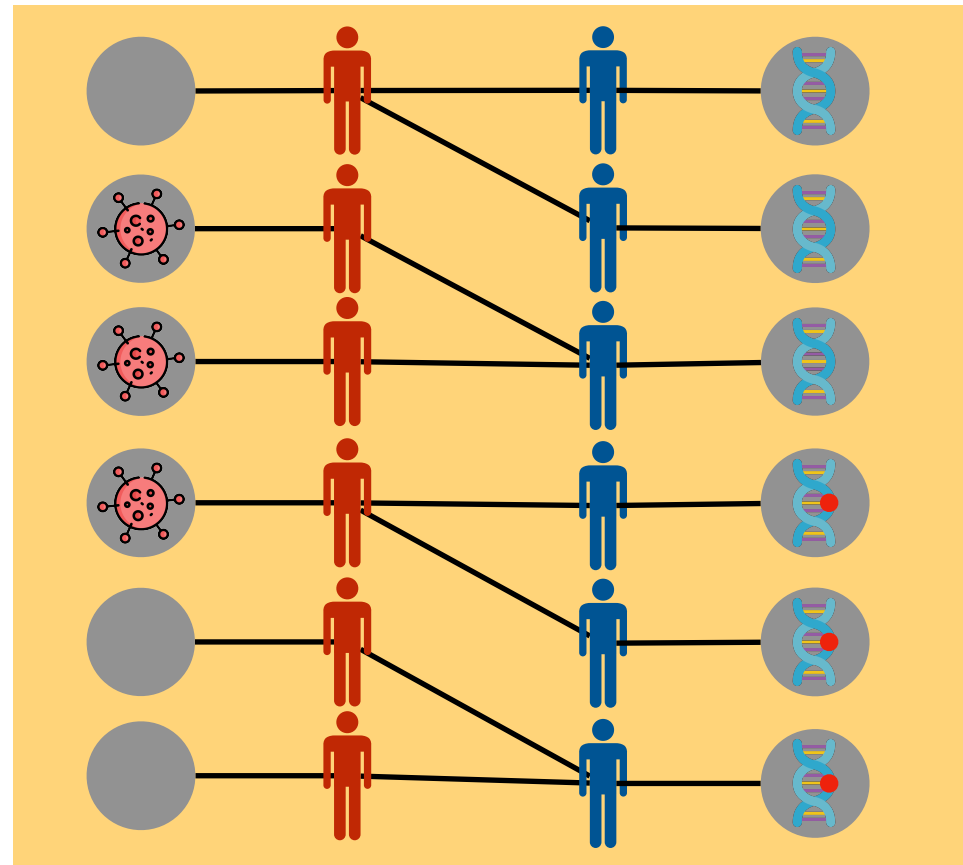
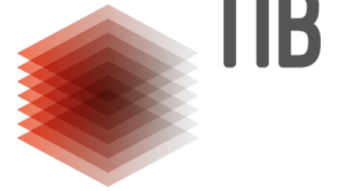
Mutation \nrightarrow Cancer

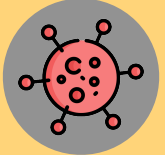



	Cancer	No Cancer
Mutation	2	2
No Mutation	2	2

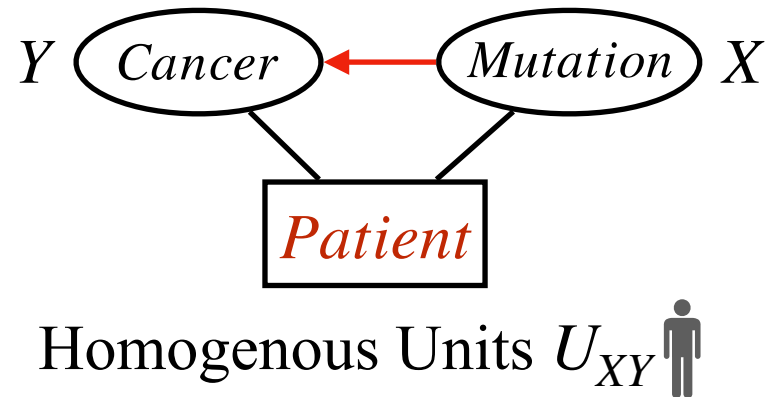
Mutation \nrightarrow Cancer

Inherited mutation

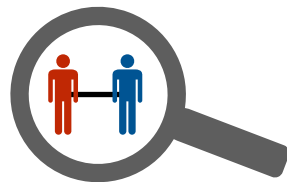
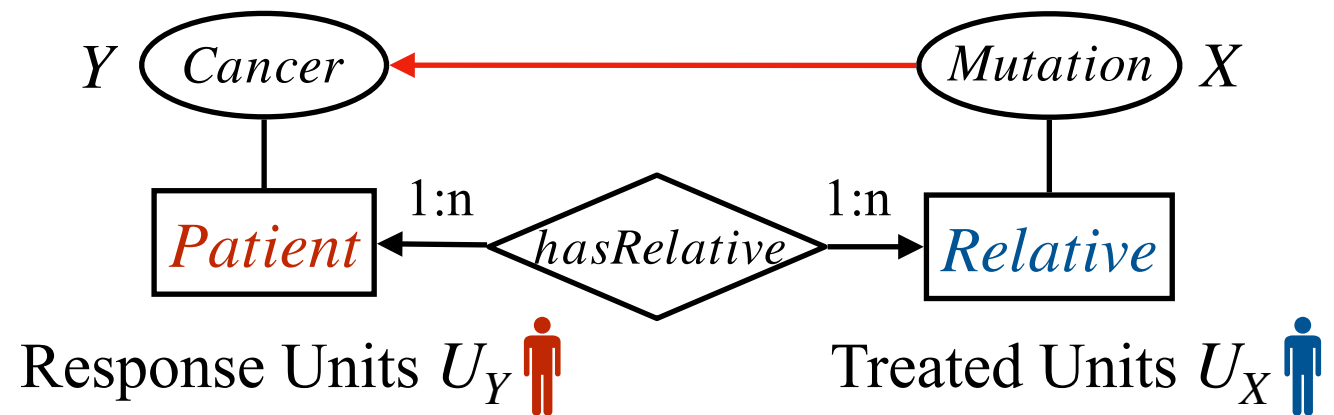
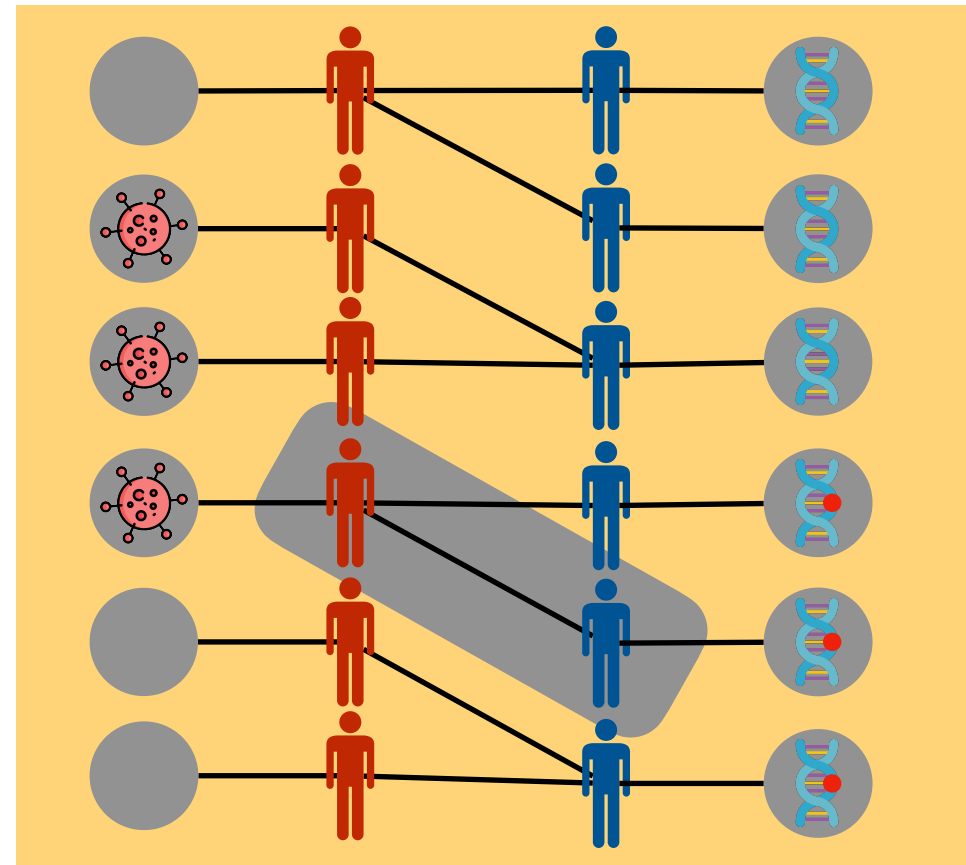


0	0
0	0
1	0
1	0
1	1
1	1
0	1
0	1



Inherited mutation

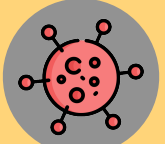



	Cancer	No Cancer
Mutation	2	2
No Mutation	2	2

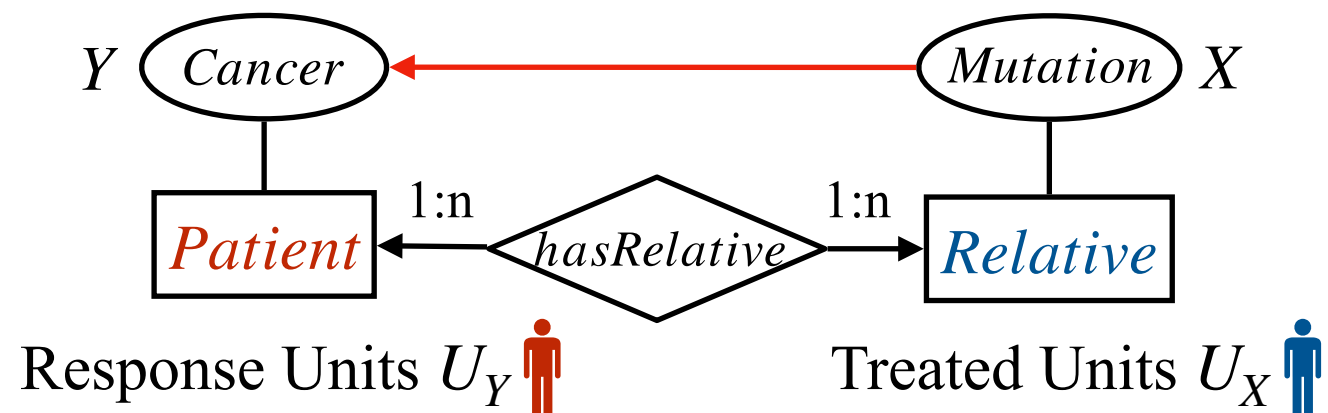
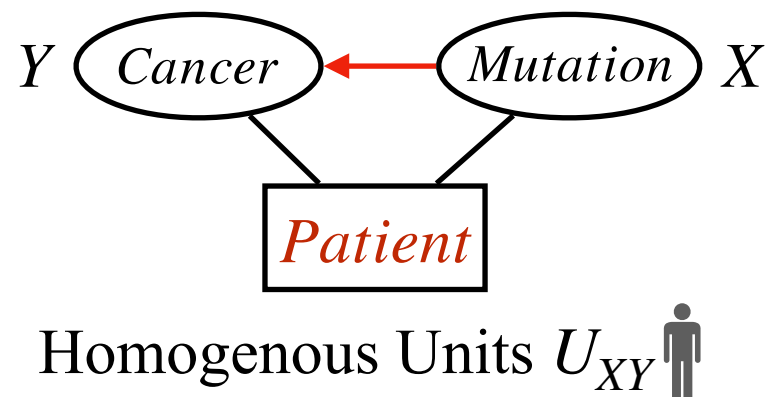
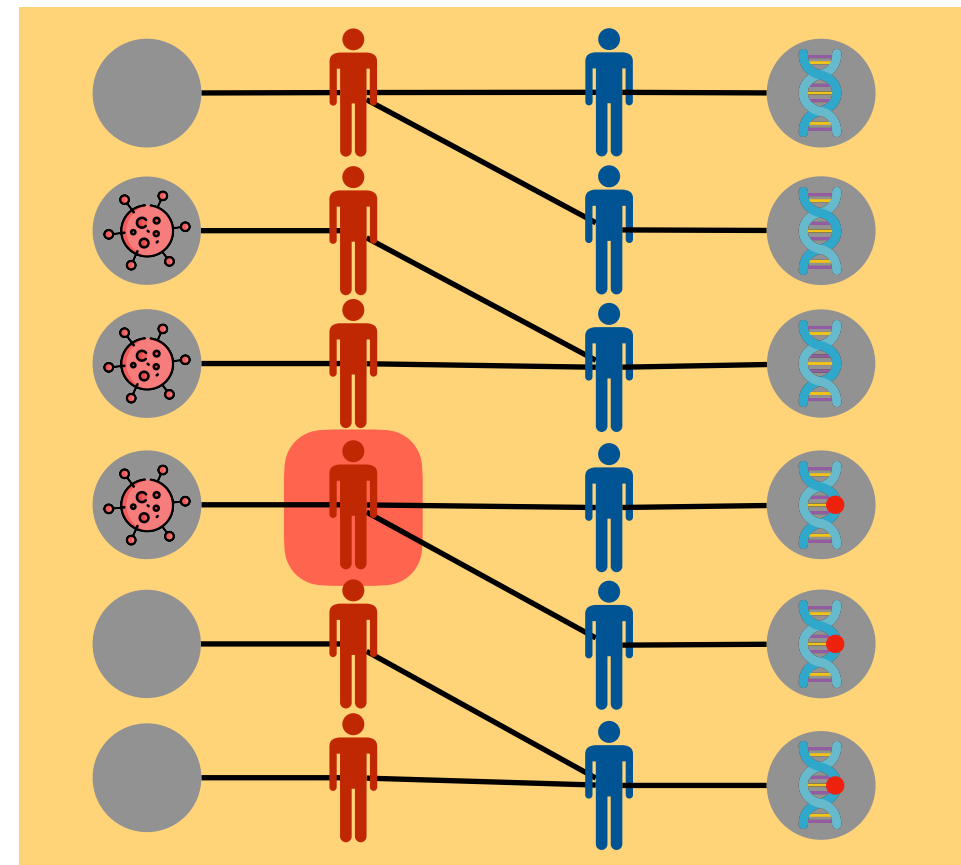
Mutation $\rightarrow \times \rightarrow$ Cancer

Perspective: a relational path \mathcal{P} ; a sequence of classes / relations.

Unit: an instance of the relational path

0	0
0	0
1	0
1	0
1	1
1	1
0	1
0	1



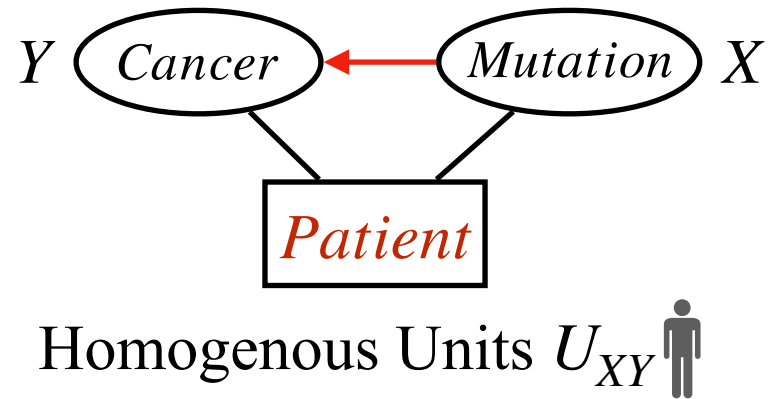
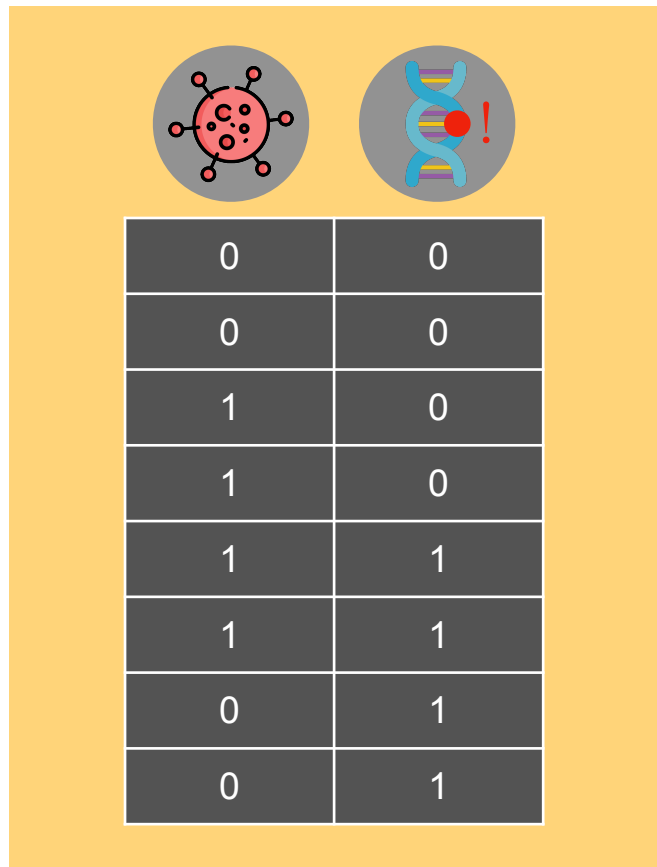
	Cancer	No Cancer
Mutation	2	2
No Mutation	2	2

Mutation \nrightarrow Cancer

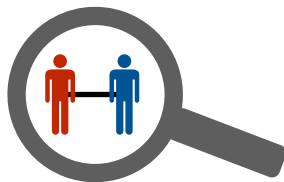
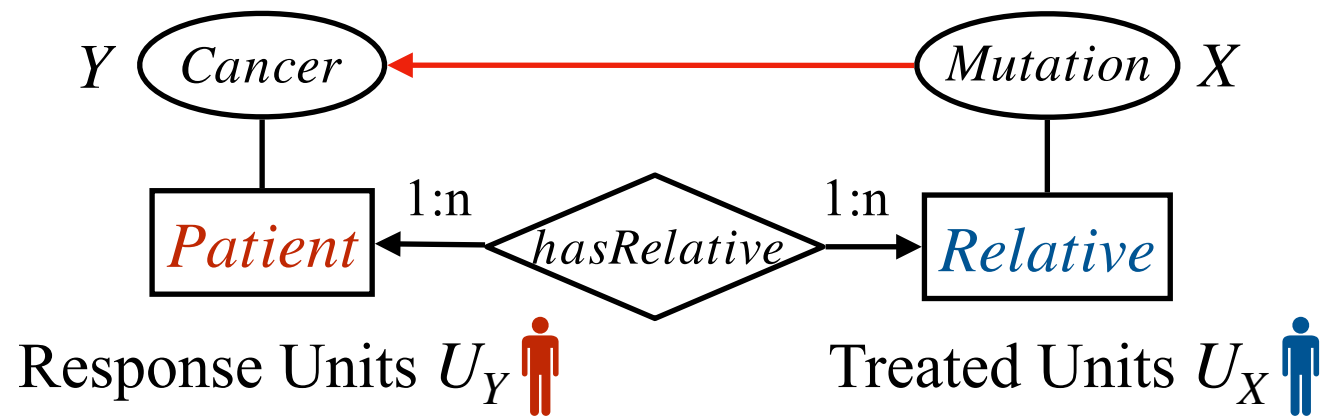
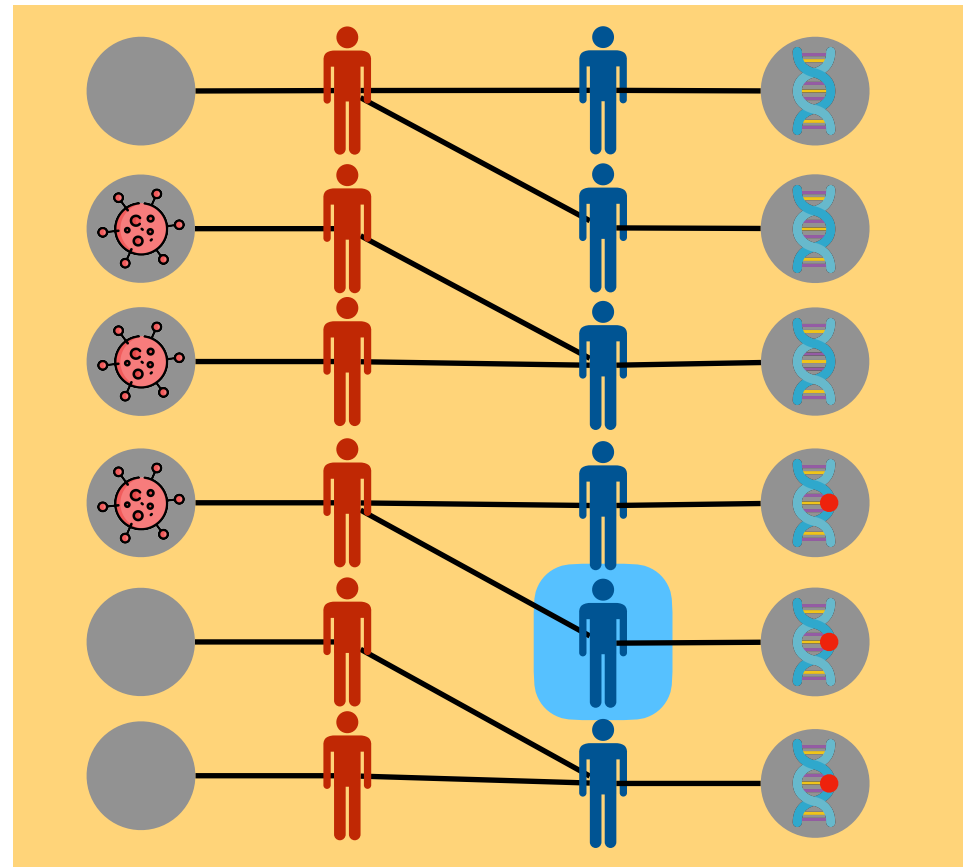


	Cancer	No Cancer
Mutation	1	2
No Mutation	2	1

Mutation $\xrightarrow{7}$ Cancer



Inherited mutation



	Cancer	No Cancer
Mutation	2	2
No Mutation	2	2

Mutation $\rightarrow \times \rightarrow$ Cancer



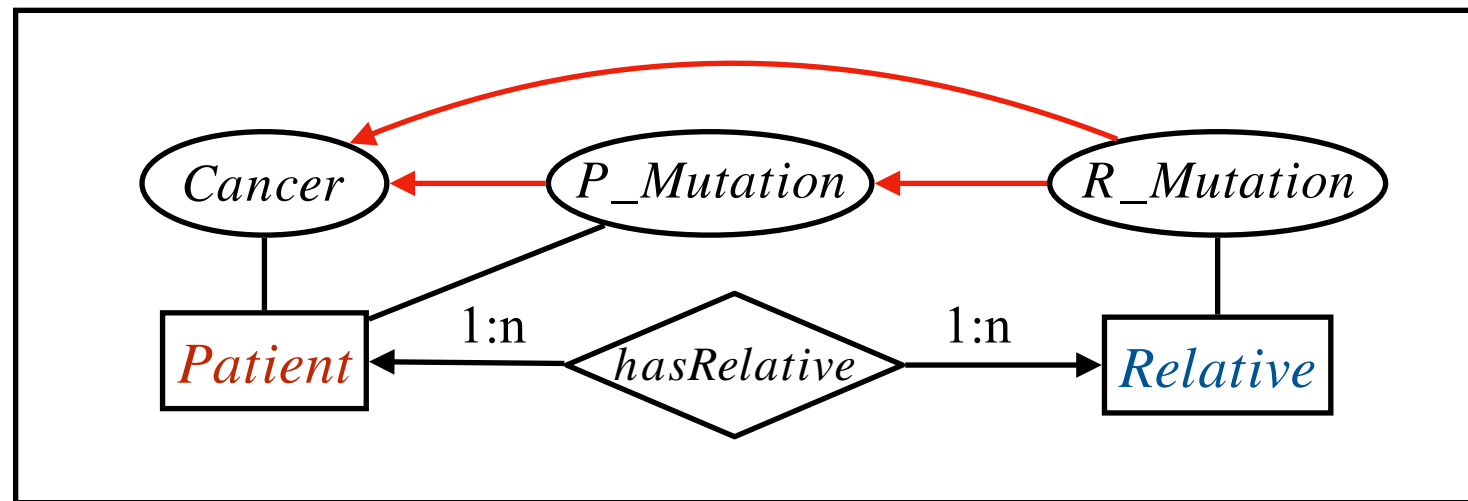
	Cancer	No Cancer
Mutation	1	2
No Mutation	2	1

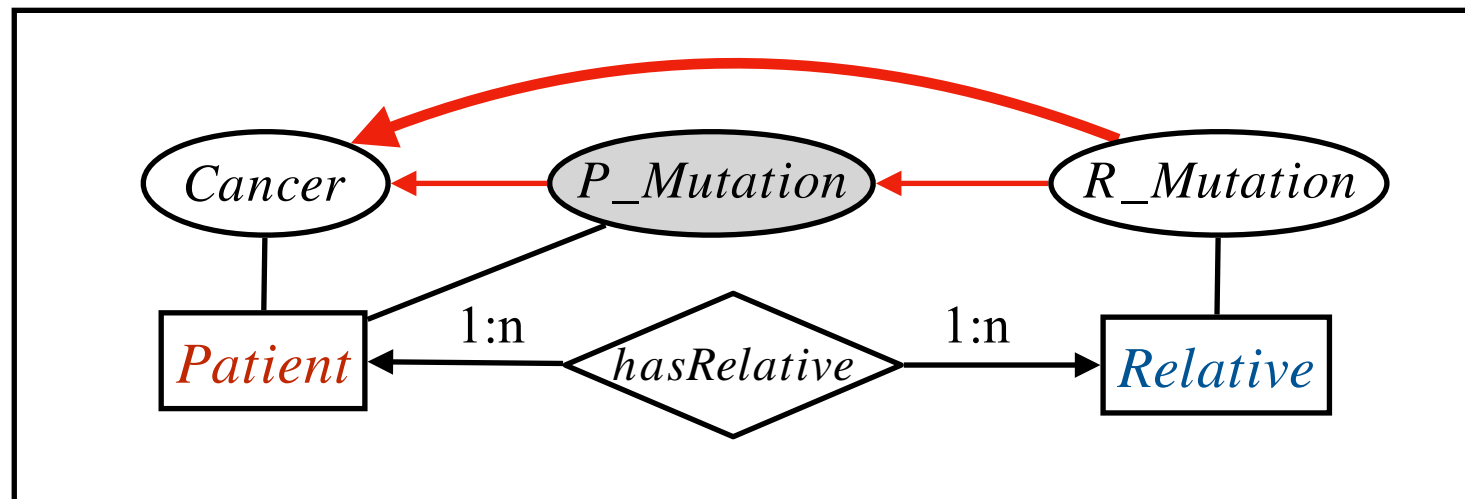
Mutation $\rightarrow \text{red line} \rightarrow$ Cancer



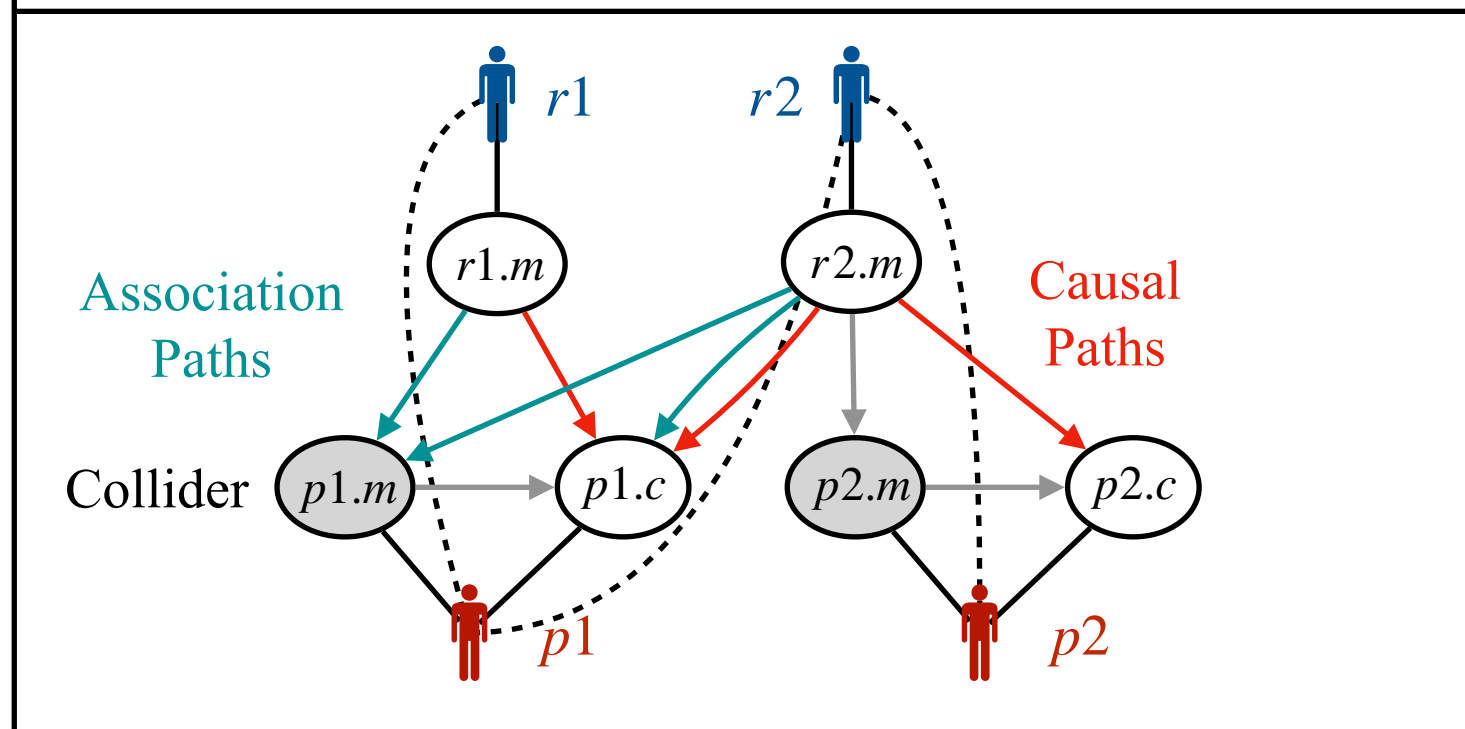
	Cancer	No Cancer
Mutation	2	1
No Mutation	1	2

Mutation $\rightarrow \text{green plus} \rightarrow$ Cancer

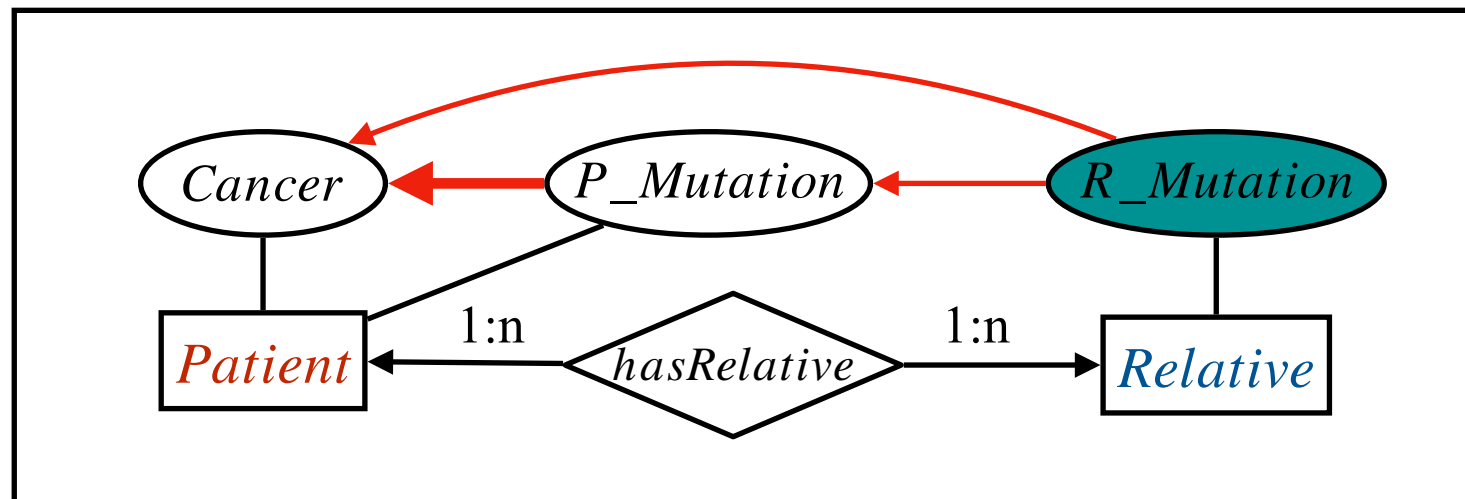




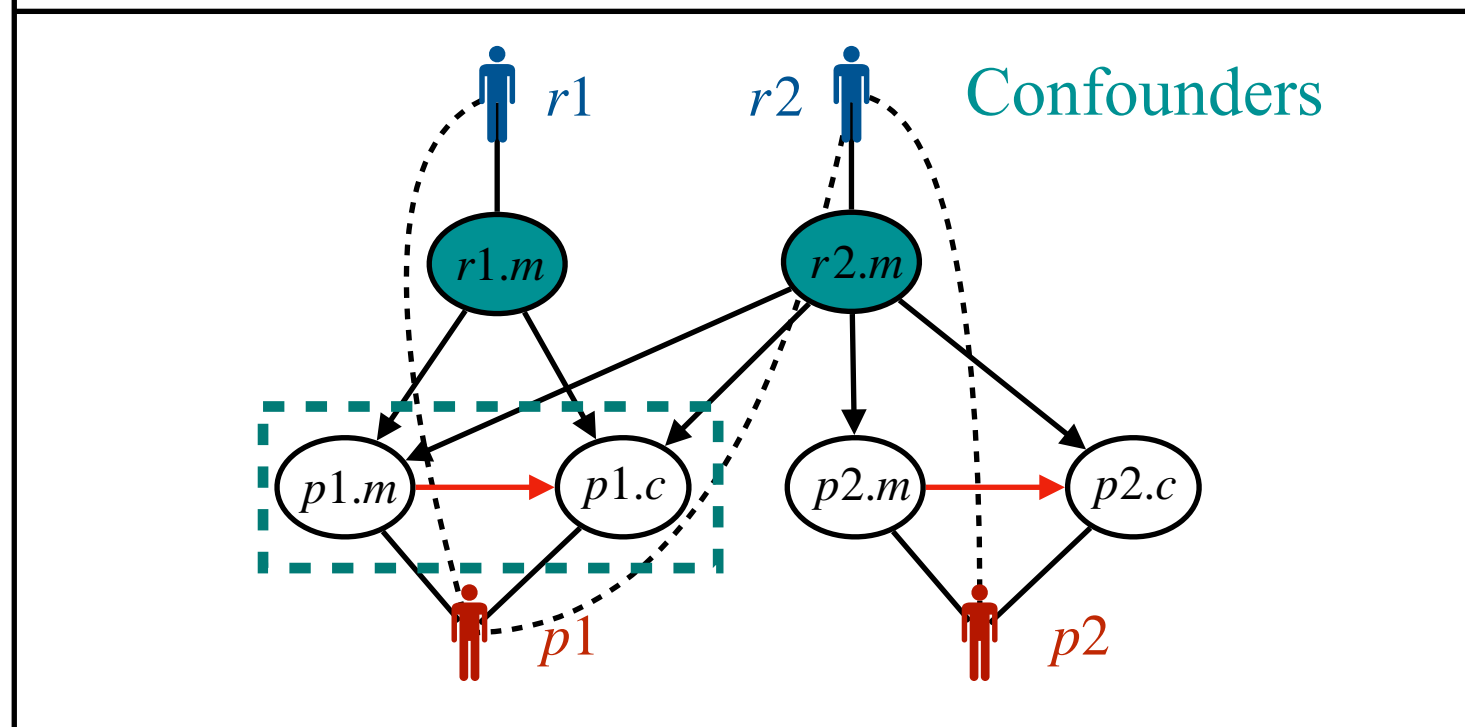
Cardinality (class : relation 1:1 **vs** 1:n)



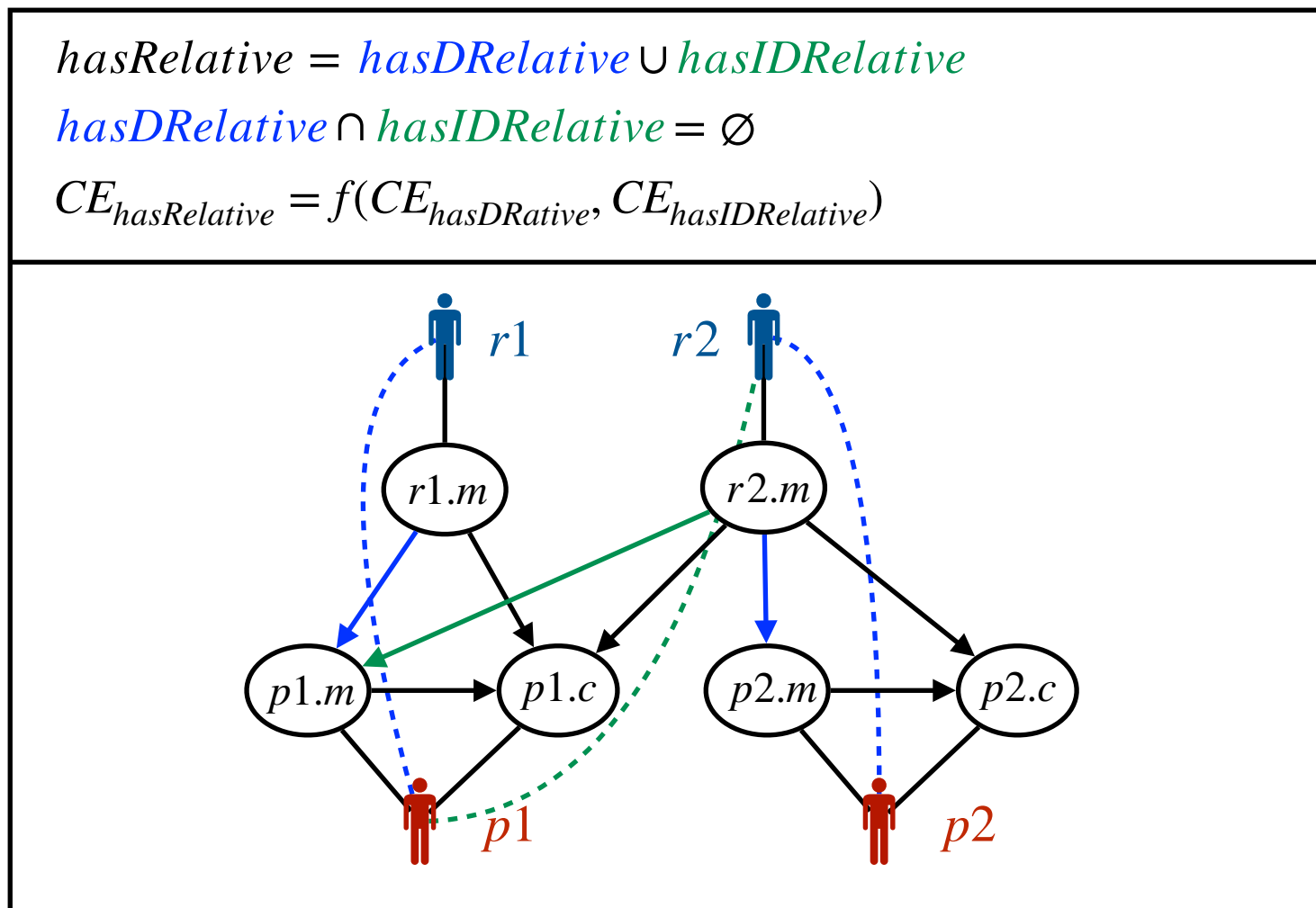
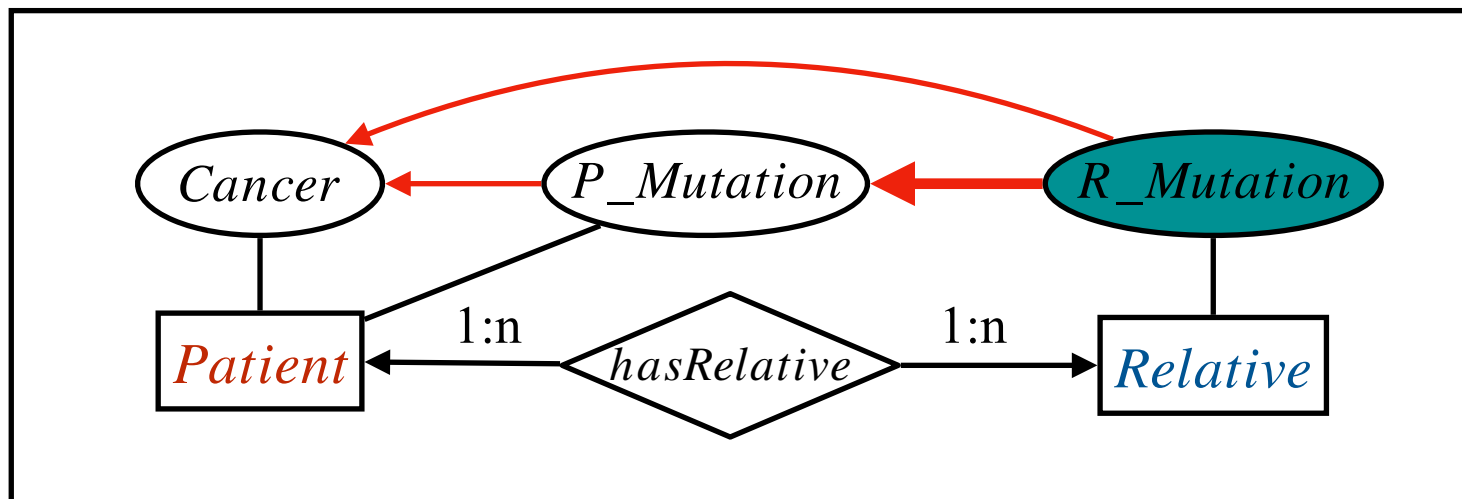
Ignoring cardinality prevents differentiating
association paths from causal paths



Cardinality (class : relation or class : attribute = 1:n)



Ignoring cardinality prevents identifying multiple confounders, or causes and effects



Ignoring subsumption, disjoint among concepts will miss the chance of sufficient inference

Related Work



- Causality over Relational Data

Causal Relational Learning (CaRL) [1]

D-seperation in Relational Data [2]

- Causality over Knowledge Graph

Causal KG [3]

Differential Causal Rule Mining [4]

[1] Babak Salimi, Harsh Parikh, Moe Kayali, Lise Getoor, Sudeepa Roy, and Dan Suciu. 2020. Causal relational learning. In Proceedings of the 2020 ACM SIGMOD International Conference on Management of Data. 241–256.

[2] Maier, Marc, Katerina Marazopoulou, and David Jensen. "Reasoning about independence in probabilistic models of relational data." *arXiv preprint arXiv:1302.4381* (2013).

[3] Jaimini, Utkarshani, and Amit Sheth. "CausalKG: Causal Knowledge Graph Explainability using interventional and counterfactual reasoning." *IEEE Internet Computing* 26.1 (2022): 43-50.

[4] Simonne, Lucas, et al. "Differential Causal Rules Mining in Knowledge Graphs." *Proceedings of the 11th on Knowledge Capture Conference*. 2021.

Related Work



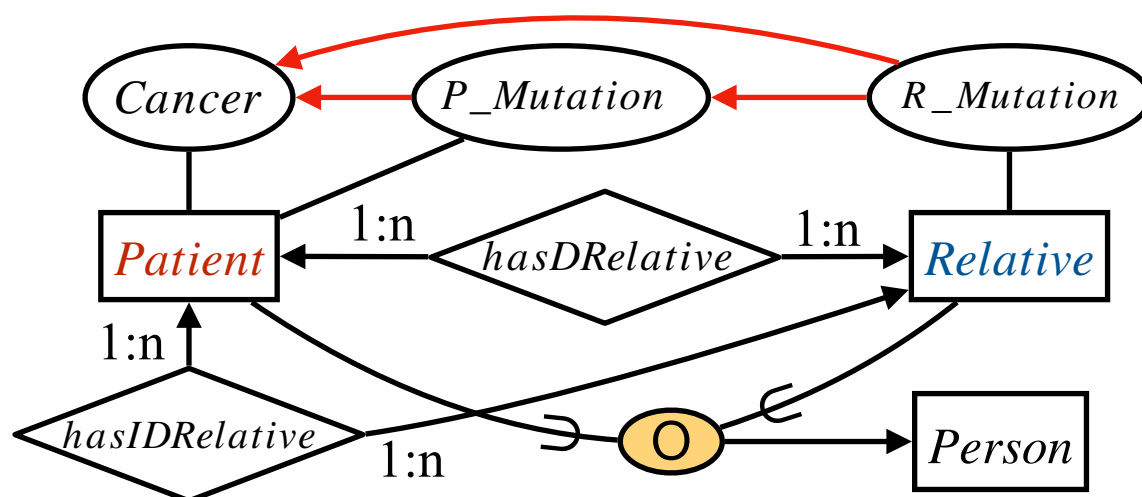
- Causality over Relational Data

Causal Relational Learning (CaRL) [1]

Relational Causal Rule of **CaRL**

$A[Y] \Leftarrow A_1[X_1], \dots, A_k[X_k] \text{ WHERE } Q(W) (Y, X_k \in W)$

$Cancer[P] \Leftarrow R_Mutation[R] \text{ WHERE } hasDRelative(P, R)$



Lacks of :

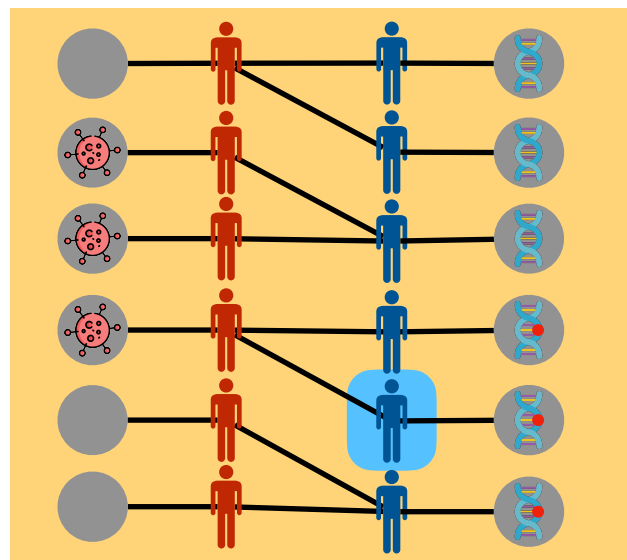
Class Disjoint	Patient - Relative
Cardinality Constraint	Patient: hasDRelative = 1:1 or 1:n ?
Integrity Constraint	hasDRelative \cap hasIDRelative = \emptyset

[1] Babak Salimi, Harsh Parikh, Moe Kayali, Lise Getoor, Sudeepa Roy, and Dan Suciu. 2020. Causal relational learning. In Proceedings of the 2020 ACM SIGMOD International Conference on Management of Data. 241–256.

Related Work

Causal Query of **CaRL**

$\text{Agg}(A[Y]) \Leftarrow A[X]? \text{ (WHEN } \underline{< cnd >} \text{ PEERS TREATED)}$



Interference between units

peer cause effect

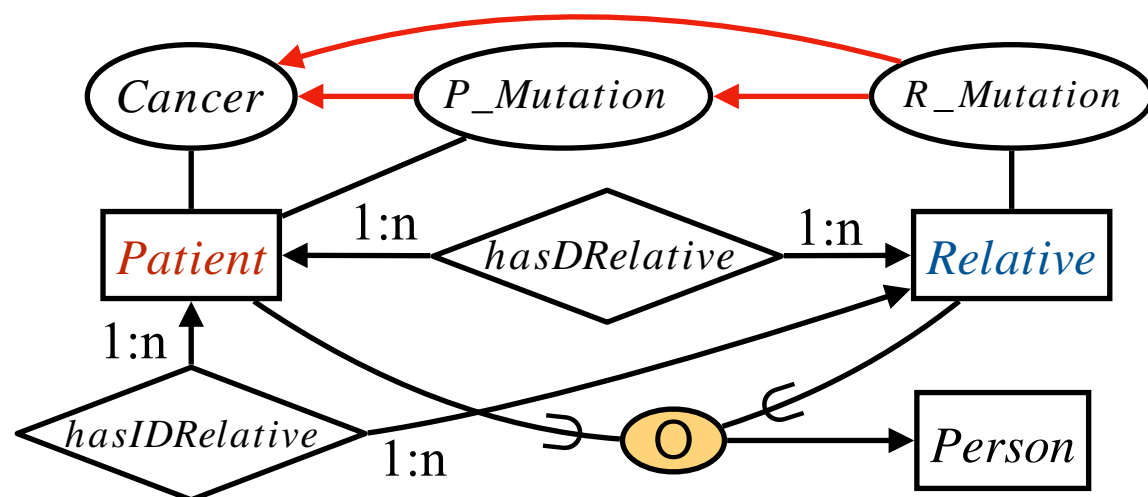
isolated cause effect



Aggregation Function: AVG, MAX, MIN, ...

Condition: Less / More than k | At (Least / Most) k | ALL | None

$\text{AVG_Cancer}[P] \Leftarrow R_Mutation[R]?$

Lacks of :



Perspective	 
The Relational Path	[Patient, hasDRelative, Relative] or [Patient, hasIDRelative, Relative]
Constraint	Relative - Patient
Peer Definition	Relative who share same patients or same Mutation?

Related Work



- Causality over Knowledge Graph

Differential Causal Rule Mining [4]

Target class & Strata: $C(X_1) \wedge C(X_2) [\wedge ST_i(X_1) \wedge ST_i(X_2)]$

Treatment: $\bigwedge_k p_k(X_1, T_1) \wedge p_k(X_2, T_2) \wedge compare(T_1, T_2)$

Outcome: $p(X_1, O_1) \wedge p(X_2, O_2) \Rightarrow \underbrace{compare(O_1, O_2)}_{\text{head}}$

$Patient(P_1) \wedge Patient(P_2) \wedge \underline{Mutation(P_1, M_1) \wedge Mutation(P_2, M_2) \wedge greatThan(M_1, M_2)}$
 $\wedge \underline{Cancer(P_1, C_1) \wedge Cancer(P_2, C_2) \Rightarrow greatThan(C_1, C_2)}$

+ : offers context (strata) where causal rule hold.
+ : allows multiple attributes as treatment.

- : lacks of consideration of semantics of KGs, e.g. cardinality, integrity constraint, etc.
- : offer fixed perspective from target class.

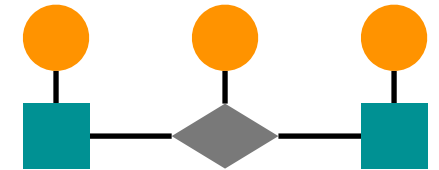
[4] Simonne, Lucas, et al. "Differential Causal Rules Mining in Knowledge Graphs." *Proceedings of the 11th on Knowledge Capture Conference*. 2021.

Problem Definition



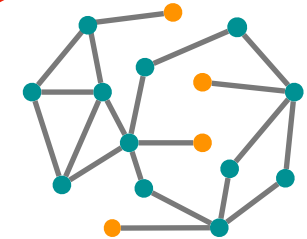
Classes Relations Attributes

Ontology: $O = \langle C, R, A \rangle$



Entities & Literals Properties Triples

Knowledge Graph: $KG = \langle V, E, T \rangle$



A surgery is only applicable
to Patients in stage I

Axioms: ζ



Problems:

1. How to represent causal relations in KGs?
2. How to formulate causal queries using semantics?

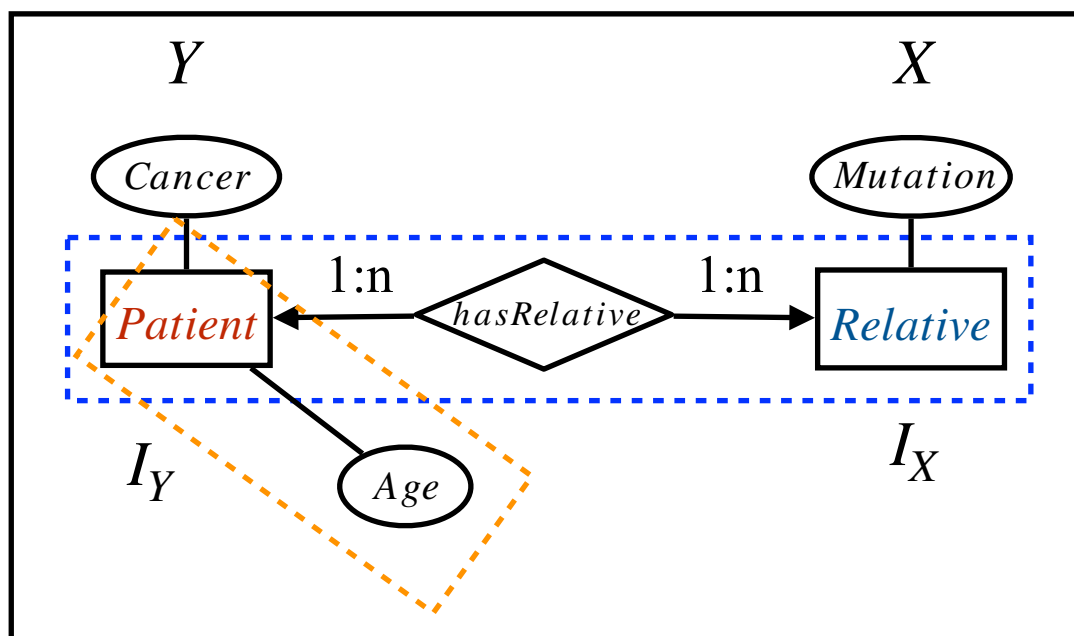
Causal Relation Representation



Ontological Causal Rule (CareKG)

$Y[I_Y] \Leftarrow X[I_X] \text{ WHERE } \underline{P(I_X, I_Y)}, \underline{CTX(I_X, I_Y)}$

Relational Path Context



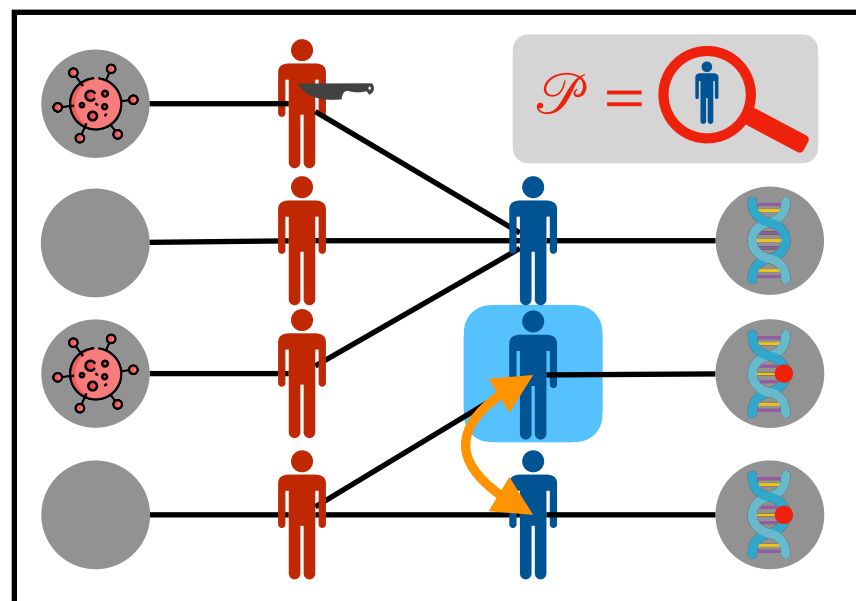
I_X is the concept (class or relation) of cause X , I_Y is the concept of effect Y

Property Path **Patient.hasAge.Age=Young** \in Context $CTX(I_X, I_Y)$

Causal Query

$\text{FUN}(Y[I_Y])$ \Leftarrow $\text{FUN}(X[I_X])$? FROM PATH P , UNDER PERSPECTIVE \mathcal{P} ,
SUBJECT TO $\langle axiom \rangle$, WHEN $\langle cnd \rangle$

FUN: (1) AVG, MAX, SUM, COUNT, COMB...; (2) DISC, REPLC

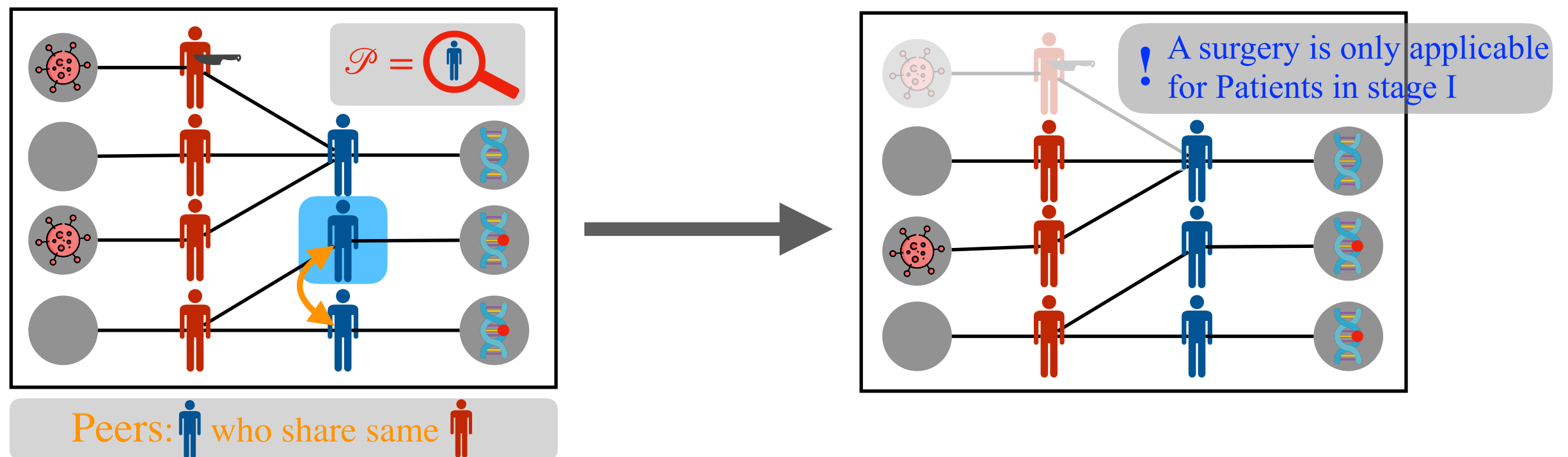


Peers:  who share same 

Causal Query

$\text{FUN}(Y[I_Y])$ \Leftarrow $\text{FUN}(X[I_X])$? FROM PATH P , UNDER PERSPECTIVE \mathcal{P} ,
SUBJECT TO $\langle axiom \rangle$, WHEN $\langle cnd \rangle$

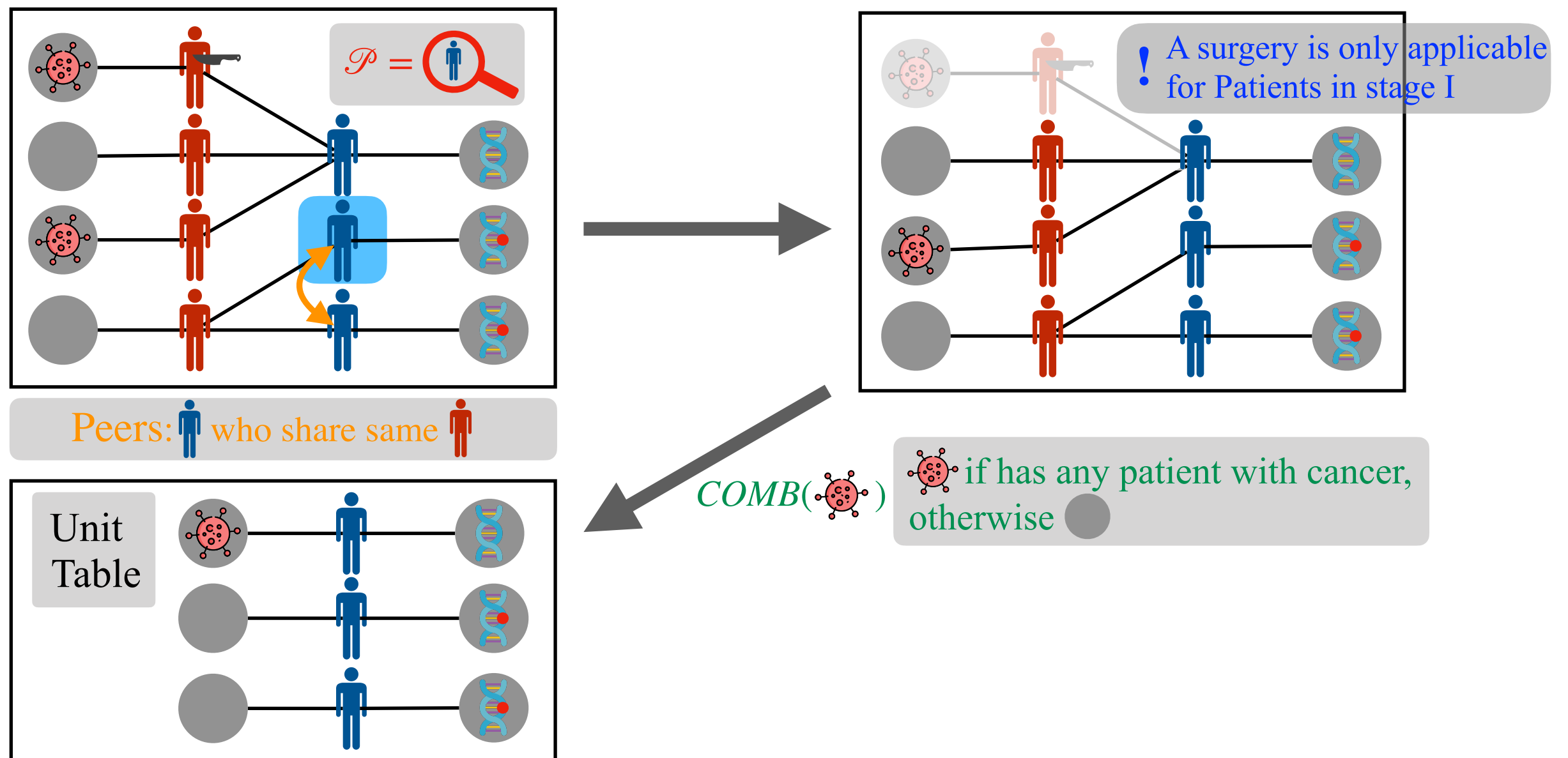
FUN: (1) AVG, MAX, SUM, COUNT, COMB...; (2) DISC, REPLC



Causal Query

$\text{FUN}(Y[I_Y]) \Leftarrow \text{FUN}(X[I_X])$? FROM PATH P , UNDER PERSPECTIVE \mathcal{P} ,
SUBJECT TO $\langle axiom \rangle$, WHEN $\langle cnd \rangle$

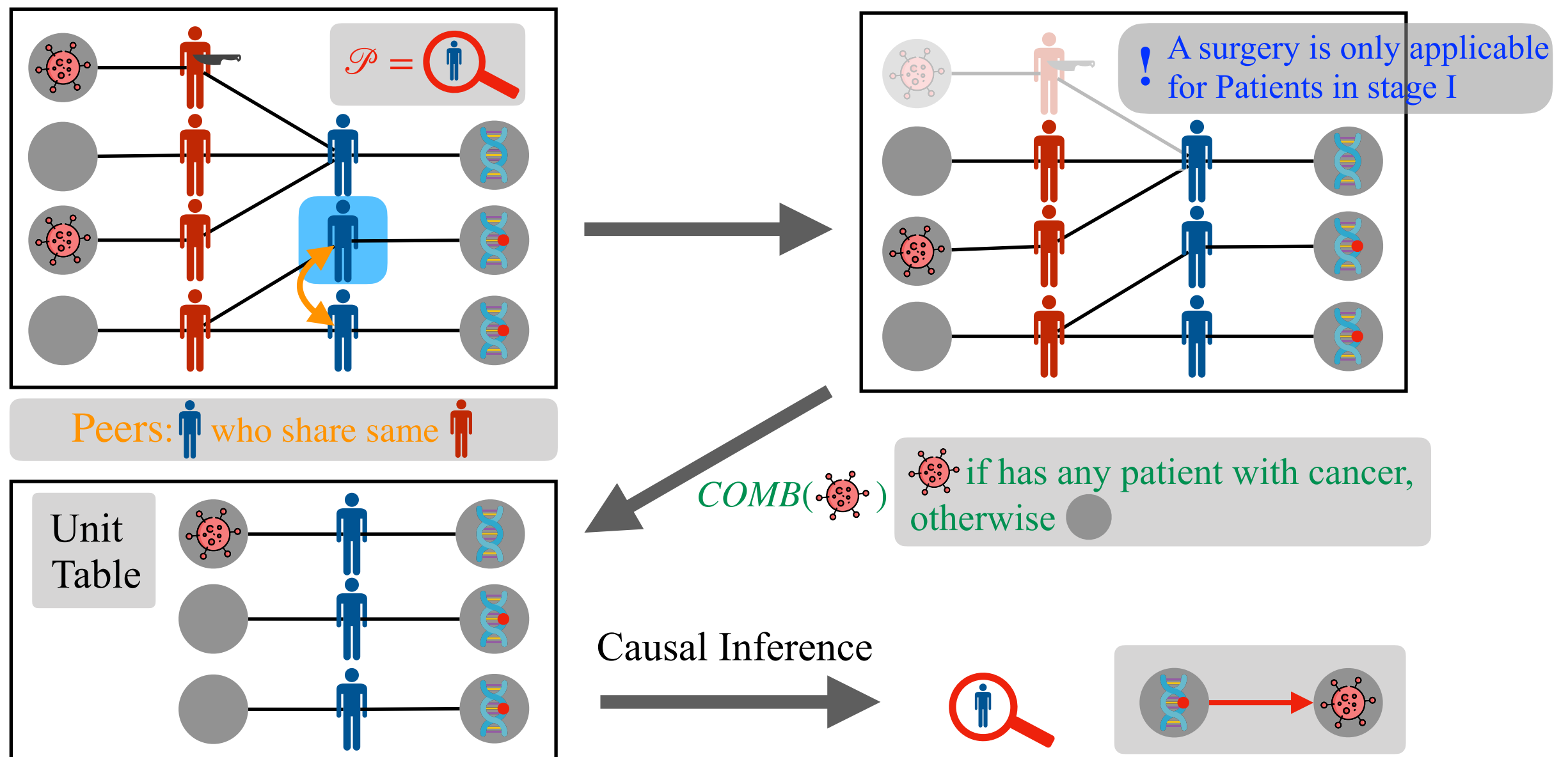
FUN: (1) AVG, MAX, SUM, COUNT, COMB...; (2) DISC, REPLC



Causal Query

$\text{FUN}(Y[I_Y]) \Leftarrow \text{FUN}(X[I_X])?$ FROM PATH P , UNDER PERSPECTIVE \mathcal{P} ,
SUBJECT TO $\langle \text{axiom} \rangle$, WHEN $\langle \text{cnd} \rangle$

FUN: (1) AVG, MAX, SUM, COUNT, COMB...; (2) DISC, REPLC



Setting of Experiment 1



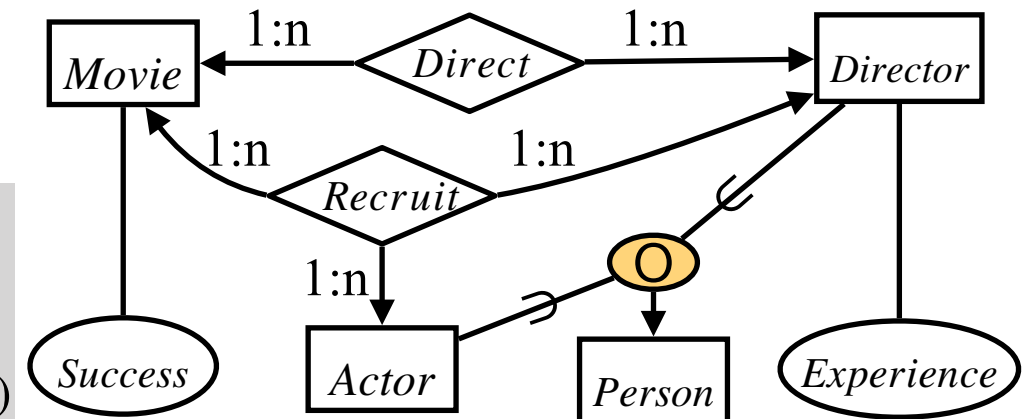
Experimental KG:

A synthetic KG “Ex - Movie”

Director	300
Actor	3043
Movie	582

$$M.Suc = 0.5 \times AVG(D_1.Exp) + 0.5 \times AVG(D_2.Exp)$$

$$(D_1 \in Director, D_2 \in Director \cap Actor)$$



Objective:

Proof the expressiveness of **CareKG** is better than **CaRL**^[1]

Causal Rules

Relational Causal Rule (**CaRL**)

$Success[M] \Leftarrow Experience[D] \text{ WHERE } Direct(D, M)$

$Success[M] \Leftarrow Experience[D] \text{ WHERE } Recruit(D, A, M)$

Ontological Causal Rule (**CareKG**)

$Success[M] \Leftarrow Experience[D] \text{ WHERE } [Director(D), Direct(D, M), Movie(M)]$

$Success[M] \Leftarrow Experience[D] \text{ WHERE } [Director(D), Recruit(D, A, M), Movie(M)]$

Results of Experiment 1



Causal Queries (CaRL)

$Success[M] \Leftarrow Experience[D]?$

$AVG_Success[M] \Leftarrow Experience[D]?$

Paths

$P_1 = [Director(D), Direct(D, M), Movie(M)]$

$P_2 = [Director(D), Recruit(D, A, M), Movie(M)]$

Causal Queries (CareKG)

$Success[M] \Leftarrow Experience[D]?$ FROM PATH P , UNDER PERSPECTIVE Direct/Recruit

$Success[M] \Leftarrow AVG(Experience[D])?$ FROM PATH P , UNDER PERSPECTIVE Movie

$AVG(Success[M]) \Leftarrow Experience[D]?$ FROM PATH P , UNDER PERSPECTIVE Director,
SUBJECT TO $\langle axiom \rangle$

(value %)	Path	Perspective		
		Director	Movie	Direct / Recruit
CareKG	P_1	44.12 (\pm 5.47)	78.70 (\pm 4.77)	41.81 (\pm 4.22)
	P_2	46.97 (\pm 5.55)	71.42 (\pm 5.82)	45.02 (\pm 0.68)
CaRL	P_1	44.07 (\pm 5.47)	-	-
	P_2	47.25 (\pm 5.56)	-	-

Table 1. perspective & path

$P = P_1, \mathcal{P} = Director$

(value %)	SUBJECT TO $\langle axiom \rangle$: I_X is		
	Director (default)	Director \cap Actor	Director - Actor
CareKG	44.12 (\pm 5.47)	67.75 (\pm 10.15)	39.73 (\pm 6.11)
CaRL	44.07 (\pm 5.47)	-	-

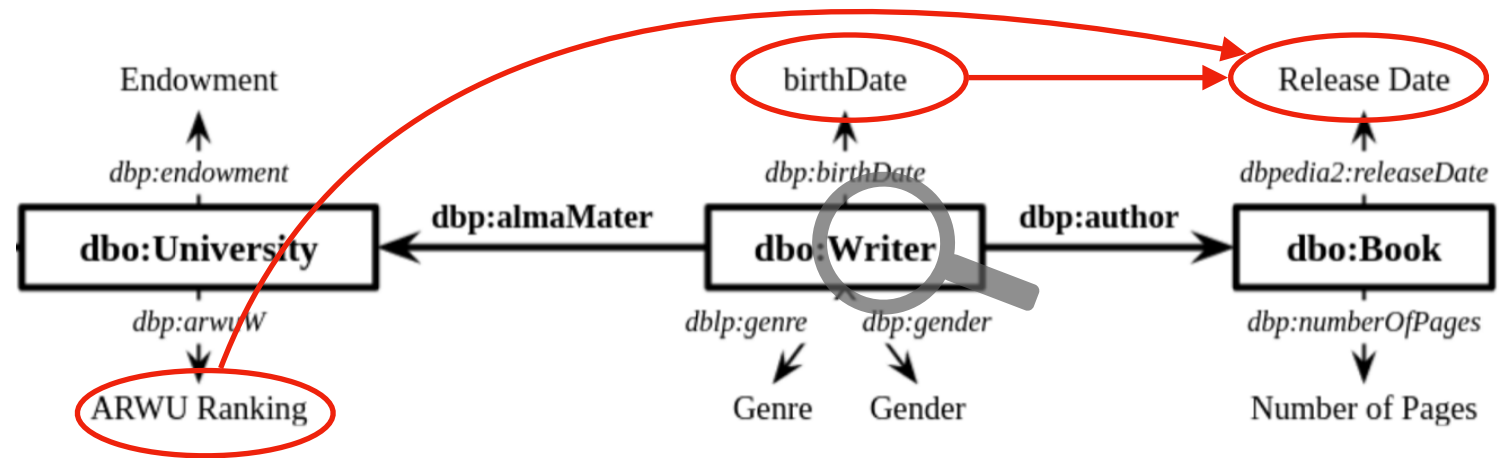
Table 2. axiom

Conclusion: CareKG has better expressiveness than CaRL

Setting of Experiment 2



Experimental KG:
A real KG “DBpediaW”



Target:

Show how CareKG works different from Differential Causal Rule Mining [4].

Ontological Causal Rule (**CareKG**)

$ReleaseDate[B] \Leftarrow birthDate[W] \text{ WHERE } [Writer(W), author(W, B), Book(B)]$

$ReleaseDate[B] \Leftarrow Ranking[U] \text{ WHERE } [University(U), almaMater(W, U),$
 $Writer(W), author(W, B), Book(B)]$

Causal Queries (**CareKG**)

$MIN(ReleaseDate[B]) \Leftarrow birthDate[W]? \text{ FROM PATH } P,$

$\text{ UNDER PERSPECTIVE } Writer(W)$

$MIN(ReleaseDate[B]) \Leftarrow AVG(Ranking[U])? \text{ FROM PATH } P,$

$\text{ UNDER PERSPECTIVE } Writer(W)$

[4] Simonne, Lucas, et al. "Differential Causal Rules Mining in Knowledge Graphs." *Proceedings of the 11th on Knowledge Capture Conference*. 2021.

Results of Experiment 2



Result from CareKG:

If a writer is 1 year younger than other, he / she publish first book 0.86 year earlier.

If a writer's university is 1 rank higher than another one's university, he / she publish book first book 0.017 year earlier.

Results from Differential Causal Rule [1]

Strata	Treatment	Effect
$genre(Fiction) \wedge gender(male) \wedge country(US)$	$univ.arwuW(i_1) \geq univ.arwuW(i_2)$	$ageFirst(i_1) \geq ageFirst(i_2)$
$genre(Fiction) \wedge country(US)$	$birthYear(i_1) \leq birthYear(i_2)$	

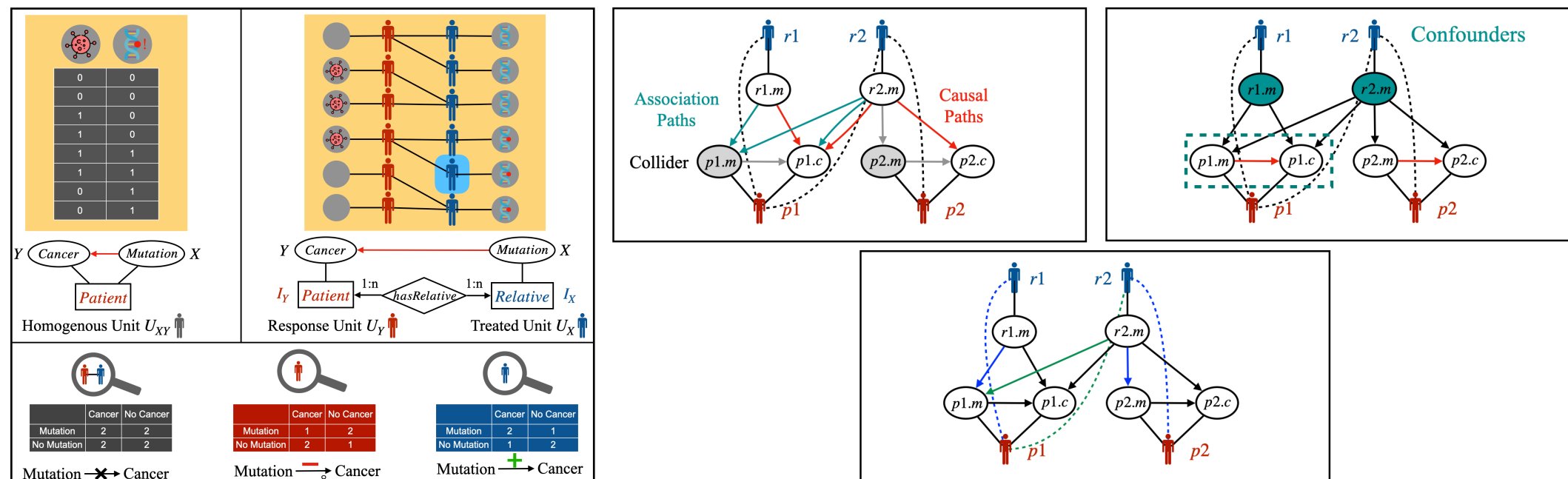
Rule 1: For male writers who writing fiction, and from US, the writer from higher ranked university publish first book earlier.

Rule 2: For writers who writing Fiction, and from US, the younger writer publish first book earlier.

[4] Simonne, Lucas, et al. "Differential Causal Rules Mining in Knowledge Graphs." *Proceedings of the 11th on Knowledge Capture Conference*. 2021.

Lessons Learned

1. Different **perspectives** allow different **unit table** definitions.
2. The classes, relations, and **metadata** upon them between them make causal inference complicated.
3. Be careful of **multi-value covariates** (causes, effects, confounders, etc)



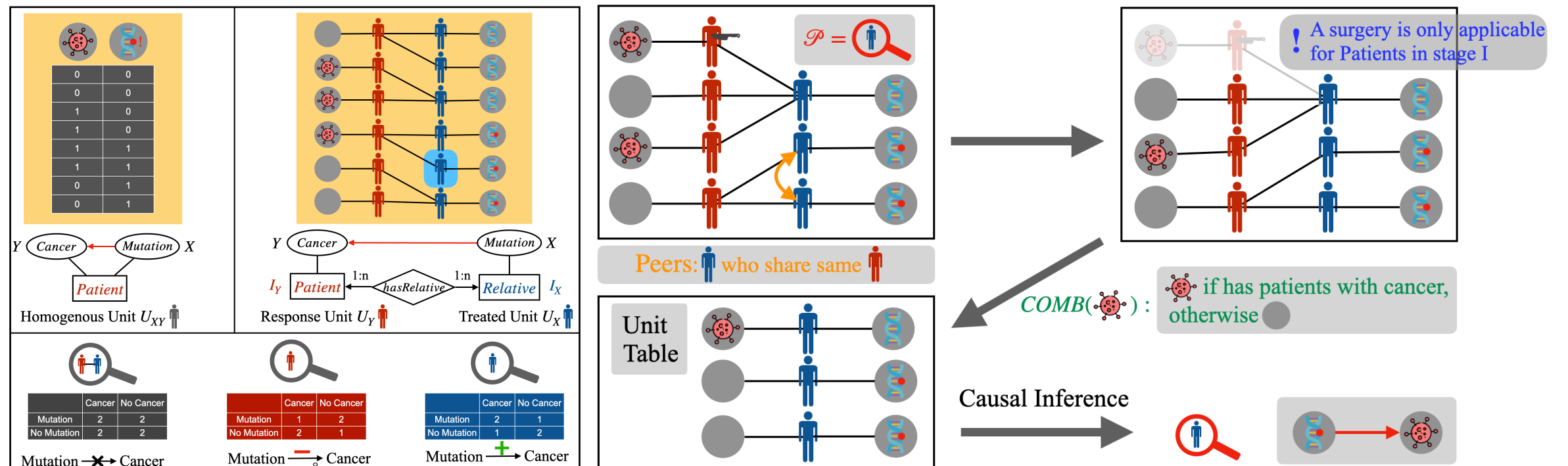
Conclusions & Future Work

Conclusions

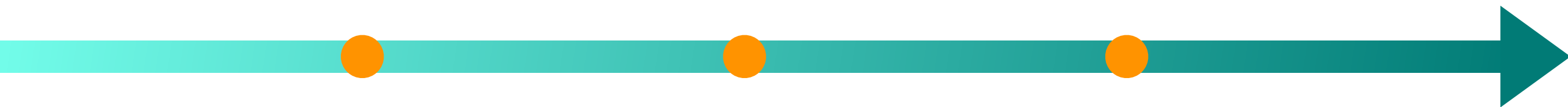
1. Offering a **new formalism** for causal query over KGs
2. Extending **causal inference** over KGs
3. Using **semantics** when doing causal queries over KGs

Future Work

1. Making causal inference **efficient** in large scale KGs
2. Studying causal inference **theory** over data structure like KGs.



Time Line



12.2022



12.2023

Causal Inference
Theory
Over KGs

12.2024

Applications over
Medical KGs

Thanks & Questions



Thanks for the **funding** from Leibniz Association
& the **travel grant** from SIGIR!

Thanks for supports of my colleagues from TrustKG project!



Hao.Huang@tib.eu



Code, Slides and Video

CareKG: <https://github.com/SDM-TIB/CareKG>



Maria.vidal@tib.eu

TrustKG Project

KG building tools: <https://github.com/SDM-TIB>

