Title: Quantum entropic causal inference

Speakers: Zubin Jacob, Vaneet Aggarwal

Collection: Causal Inference & Quantum Foundations Workshop

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Abstract: The class of problems in causal inference which seeks to isolate causal correlations solely from observational data even without interventions has come to the forefront of machine learning, neuroscience and social sciences. As new large scale quantum systems go online, it opens interesting questions of whether a quantum framework exists on isolating causal correlations without any interventions on a quantum system. We put forth a theoretical framework for merging quantum information science and causal inference by exploiting entropic principles. At the root of our approach is the proposition that the true causal direction minimizes the entropy of exogenous variables in a non-local hidden variable theory. The proposed framework uses a quantum causal structural equation model to build the connection between two fields: entropic causal inference and the quantum marginal problem. First, inspired by the definition of geometric quantum discord, we fill the gap between classical and quantum conditional density matrices to define quantum causal models. Subsequently, using a greedy approach, we develop a scalable algorithm for quantum entropic causal inference unifying classical and quantum causality in a principled way. We apply our proposed algorithm to an experimentally relevant scenario of identifying the subsystem impacted by noise starting from an entangled state. This successful inference on a synthetic quantum dataset can have practical applications in identifying originators of malicious activity on future multi-node quantum networks as well as quantum error correction. As quantum datasets and systems grow in complexity, our framework can play a foundational role in bringing observational causal inference from the classical to the quantum domain.

Quantum causal inference in the presence of hidden common causes: An entropic approach
Mohammad Ali Javidian, Vaneet Aggarwal, and Zubin Jacob
Phys. Rev. A **106**, 062425 (2022)

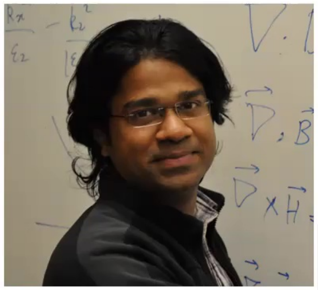
# QUANTUM ENTROPIC CAUSAL INFERENCE


Vaneet Aggarwal

Joint with:



Mohammad Ali Javidian


Zubin Jacob

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# CAUSAL RELATION : STRUCTURAL EQUATION


- X is a cause of Y if the change of X causes a change in the distribution of Y.
- More precisely, $P(Y < y|X = x) = f(x, y, E)$, where E is some exogenous random variable.

$$Y = f(X) + E$$ (additive noise models)

Kocaoglu, M., Dimakis, A., Vishwanath, S., & Hassibi, B. (2017, February). Entropic causal inference. In *Proceedings of the AAAI Conference on Artificial Intelligence* (Vol. 31, No. 1).

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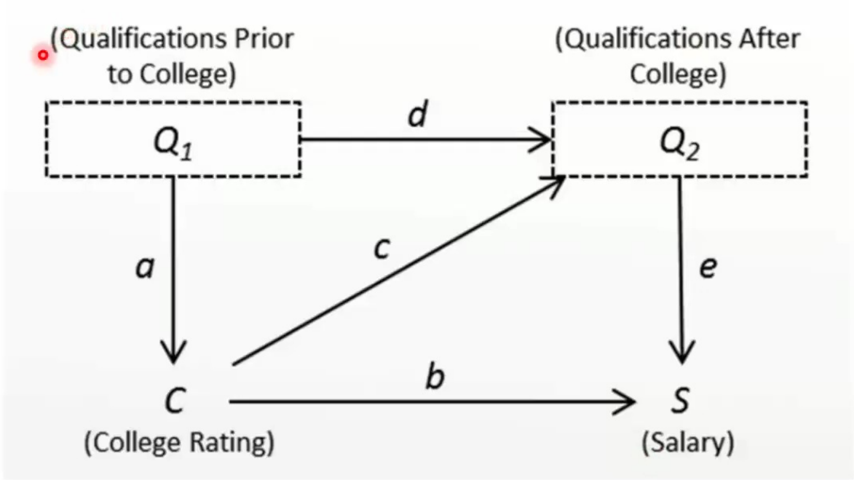
# CAUSAL GRAPHS




- Causal relation on each edge
- Different exogenous random variables are independent

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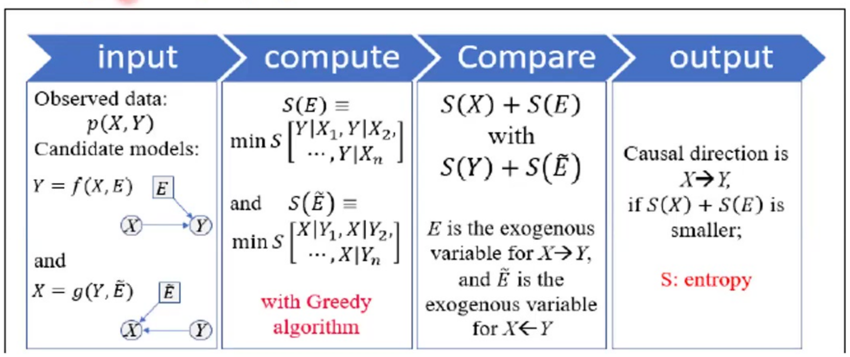
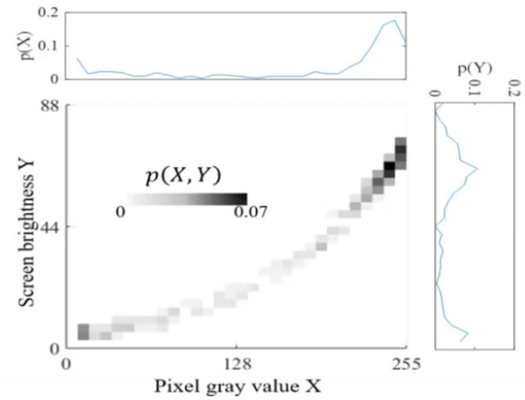
# CLASSICAL ENTROPIC CAUSAL INFERENCE

- Use only observational data
- Entropic argument


**Assumption 1.** *Entropy of the exogenous variable $E$ is small in the true causal direction.*




Example from classical cause-effect repository

Kocaoglu, M., Dimakis, A., Vishwanath, S., & Hassibi, B. (2017, February). Entropic causal inference. In *Proceedings of the AAAI Conference on Artificial Intelligence* (Vol. 31, No. 1).

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# OUTLINE

- Defining Quantum Causality between nodes
- Finding Causal Direction
- Application to Tubingen dataset

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# GENERALIZING STRUCTURAL EQUATION BETWEEN NODES


- Classical Definition:

$$P(Y < y|X = x) = f_y(x, E)$$

- Quantum Causality => structural equations

$$\widetilde{\rho}_{Y|X=|x\rangle^{obs}} = f(|x\rangle^{obs}, \rho_E)$$

$$\rho_{A|B=|b\rangle} = \frac{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}}{trace\{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}\}}$$

Instance Conditional Observational Density Matrix

Observed data

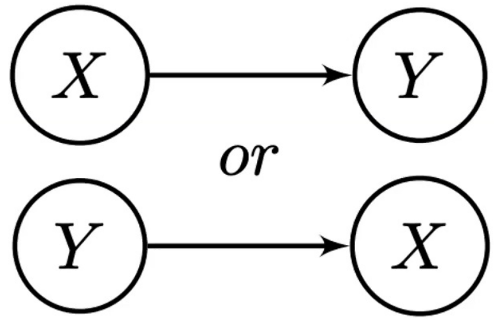
**Non-local**
**Hidden variable theory**

# BEYOND CLASSICAL CAUSALITY

- Quantum Causality

$$\rho_{Y|X=|x\rangle^{obs}} = f(|x\rangle^{obs}, \rho_E)$$

$$\rho_{A|B=|b\rangle} = \frac{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}}{trace\{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}\}}$$




- Assumption: The entropy of exogenous variable is lower in the causal direction.

- **Thus: the key is to estimate entropy of exogenous variable in both directions and compare for direction**

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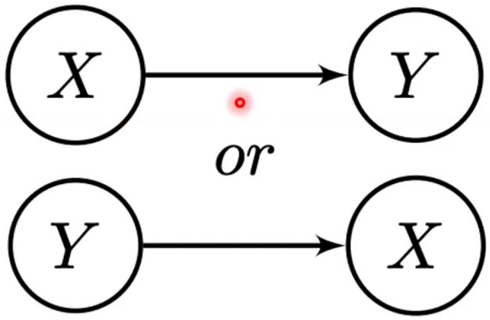
# EXOGENOUS VARIABLE

- Quantum Causality

$$\rho_{Y|X=|x\rangle^{obs}} = f(|x\rangle^{obs}, \rho_E)$$

$$\rho_{A|B=|b\rangle} = \frac{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}}{trace\{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}\}}$$




- Assumption: The entropy of exogenous variable is lower in the causal direction.

$$\rho_{U_i} = \rho_{Y|X=|x_i\rangle} = f(|x_i\rangle, \rho_E) = f_{|x_i\rangle}(\rho_E)$$

- The exogenous variable can be found as the density matrix U which reduces corresponding Ui on the relevant projection. Intuition from classical:

$$S(\rho_E) = \underbrace{S(\rho_E|\rho_{U_1,\ldots,U_n})}_{\geq 0} + S(\rho_{U_1,\ldots,U_n}) - \underbrace{S(\rho_{U_1},\ldots,\rho_{U_n}|\rho_E)}_{=0}$$

$$\geq S(\rho_{U_1,\ldots,U_n}).$$

*Work in progress*

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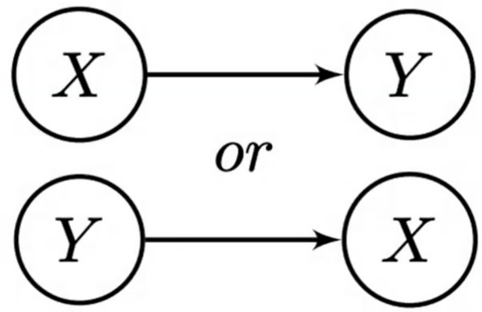
# QUANTUM CAUSALITY DIRECTION

- Quantum Causality

$$\rho_{Y|X=|x\rangle^{obs}} = f(|x\rangle^{obs}, \rho_E)$$

$$\rho_{A|B=|b\rangle} = \frac{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}}{trace\{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}\}}$$

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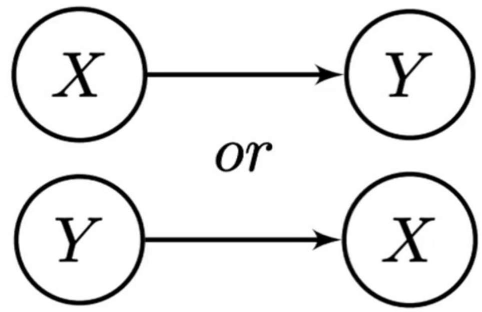


- Assumption: The entropy of exogenous variable is lower in the causal direction.

$$\rho_{U_i} = \rho_{Y|X=|x_i\rangle} = f(|x_i\rangle, \rho_E) = f_{|x_i\rangle}(\rho_E)$$

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$$\geq S(\rho_{U_1,\ldots,U_n}).$$

*Work in progress*

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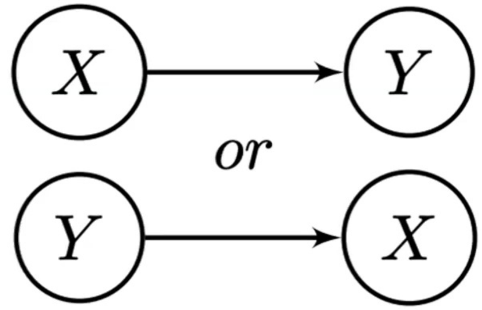
# EXOGENOUS VARIABLE




- Quantum Causality

$$\rho_{Y|X=|x\rangle^{obs}} = f(|x\rangle^{obs}, \rho_E)$$

- Assumption: The entropy of exogenous direction.

$$\rho_{U_i} \triangleq \rho_{Y|X=|x_i\rangle} = f(|x_i\rangle, \rho_E) = f_{|x_i\rangle}(\rho_E)$$

- Finding Exogenous random variable:

$$S(\rho_{E^*}) = \min_{\rho_{U_1,\ldots,U_n}} S(\rho_{U_1}, \ldots, \rho_{U_n})$$
$$\text{subject to } \mathbf{Tr}_{U_1,\ldots,U_{i-1},U_{i+1},\ldots,U_n}(\rho_{U_1,\ldots,U_n}) = \rho_{U_i}, \forall i = 1, \ldots, n.$$

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# EXOGENOUS VARIABLE

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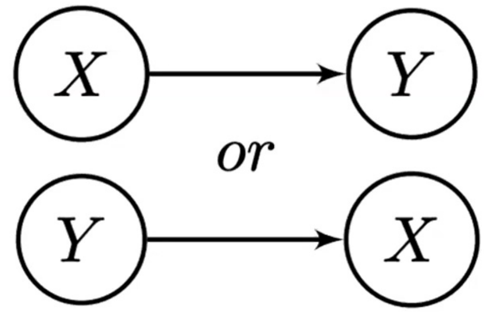


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- Greedy Algorithm is proposed to solve the optimization.

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# GREEDY ALGORITHM

- Assumption: The entropy of exogenous variable is lower in the causal direction.

**Input:** Density matrices of quantum systems $A$ and $B$ i.e., $\rho_A$ and $\rho_B$ of the size $m$-by-$m$ and $n$-by-$n$, respectively.

**Output:** Minimum entropy $S(\rho_E)$ of the joint density matrix.

/* Step 1:Compute eigenvalues of $\rho_A$ and $\rho_B$ */

$p_A = eig(\rho_A)$;

$q_B = eig(\rho_B)$;

/* Step 2: Apply Joint Entropy Minimization Algorithm (Kocaoglu et al., 2017b) on $p_X$ and $q_Y$. */

$e = [\quad]$;

Initialize the matrix $M_{ij} = 0, i = 1, \ldots, m, j = 1, \ldots, n$;

Initialize $r = 1$;

**while** $r > 0$ **do**

  e=[e,r];

  $(\{p_A, q_B\}, r)$ = **UpdateRoutine**$(\{p_A, q_B\}, r)$

**end**

**UpdateRoutine**$(\{p_A, q_B\}, r)\{$

$i = \text{argmax}_k\{p_k\}$;

$j = \text{argmax}_k\{q_k\}$;

$Mij = \min\{p_i, qj\}$;

$p_i = p_i - M_{ij}$;

$q_i = q_i - M_{ij}$;

$r = r - M_{ij}$;

$\}$

$S(\rho_E) = -\sum_k e_k \log(e_k)$;

**return** $S(\rho_E)$.

# QUANTUM CAUSALITY BETWEEN NODES


- Quantum Causality

$$\rho_{Y|X=|x\rangle^{obs}} = f(|x\rangle^{obs}, \rho_E)$$

$$\rho_{A|B=|b\rangle} = \frac{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}}{trace\{\boldsymbol{Tr}_B\{\rho_{BA} \star |b\rangle\langle b|\}\}}$$

- Example:

$$\rho_{XY} = \frac{1}{2}(1-p)(|00\rangle\langle 00| + |11\rangle\langle 11|) + \frac{1}{2}p(|01\rangle\langle 01| + |10\rangle\langle 10|)$$

- (X,Y) is prepared in superposition state, and 2nd qubit is passed over a bit-flip channel.

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- Quantum Causality

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- (X,Y) is prepared in superposition state, and 2nd qubit is passed over a bit-flip channel.

$$\rho_{Y|X=|x\rangle} = (1-p)|x\rangle\langle x| + p(\sigma_X|x\rangle)(\sigma_X|x\rangle)^\dagger$$

$$\rho_{Y|X=|x\rangle} = f(|x\rangle, \rho_E) = 2M\rho_E M^\dagger$$

$$M = |x\rangle^\dagger \otimes I_2, \; \rho_E = \tfrac{1}{2}diag([1-p, p, p, 1-p])$$

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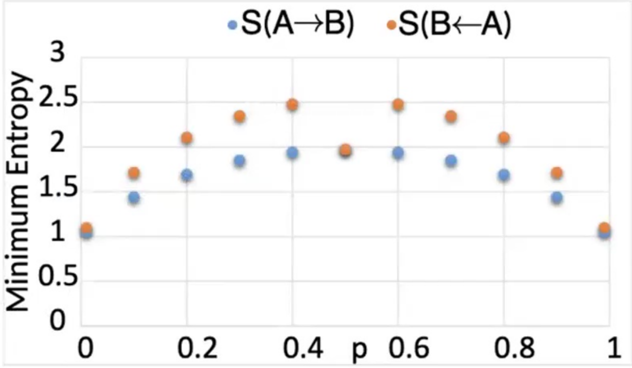
# EVALUATIONS

- Joint system (A,B) is prepared in a superposition of two states, and the sub-system B is transmitted over noisy channel.
- After transmission joint system is

$$\begin{cases} (|A_1\rangle|B_1\rangle)(|A_1\rangle|B_1\rangle)^\dagger & q(1-p) \\ (|A_1\rangle|B_2\rangle)(|A_1\rangle|B_2\rangle)^\dagger & qp \\ (|A_2\rangle|B_1\rangle)(|A_2\rangle|B_1\rangle)^\dagger & (1-q)p \\ (|A_2\rangle|B_2\rangle)(|A_2\rangle|B_2\rangle)^\dagger & (1-q)(1-p) \end{cases}$$




- For q = 0.4, we get A-> B as the better explanation.
- Can also do depolarizing channel with similar results.

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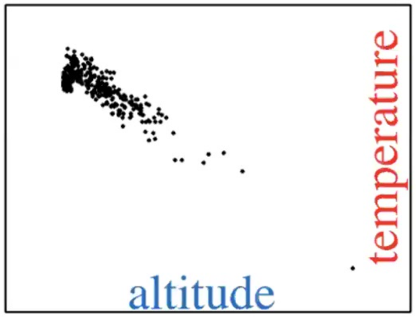
# EVALUATIONS ON TUBINGEN DATA




We have generalized to common confounder

| Algorithm | True Positive | False Positive | False Negative | Accuracy |
|---|---|---|---|---|
| QInferGraph ($\alpha = 0.2, T = 0.005$) | **0.83** | 0 | **0.17** | **0.83** |
| Classical **InferGraph** ($\alpha = 0.8, T = 0.001$) | 0.32 | 0 | 0.68 | 0.32 |
| Classical **InferGraph** ($\alpha = 0.7, T = 0.001$) | 0.49 | 0 | 0.51 | 0.49 |

- Quantum Approach gives better accuracy on real dataset.

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# CONCLUSIONS

- Defining Quantum Causality between nodes
- Finding Causal Direction
- Application to Tubingen dataset

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