

Closing the Problem of Classical-Quantum Gaps in Causal Structures: Which causal structures of up to six nodes support non-classical quantum correlations?

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Outline

- 1 Introduction: Understanding Causality
- 2 Main Result: The Causal Structure G1
- 3 Generalization: Other Causal Structures
- 4 Completing the Classification
- 5 Conclusions

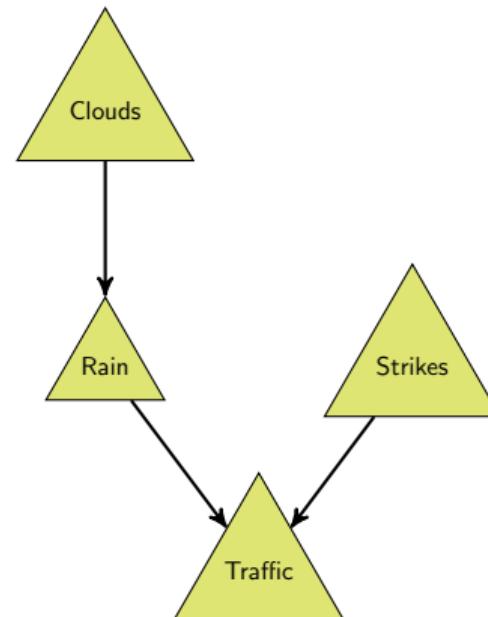
Motivation: Why Study Causality?

Everyday causality:

- Clouds cause rain
- Rain causes traffic delays
- Strikes cause traffic delays

Key question:

Can we represent these relationships formally?



Goal

Develop a mathematical framework to represent and analyze causal relationships.

Causal Structures: Directed Acyclic Graphs (DAGs)

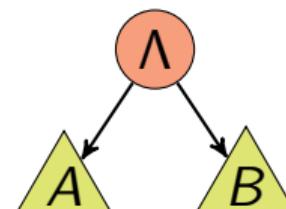
Definition

A **causal structure** (or DAG) is a directed acyclic graph where:

- **Nodes** represent variables (events, measurements)
- **Directed edges** represent *possible* direct causal influences
- **No cycles** (acyclic): cannot return back to the same node following a (directed) path formed by directed edges.

Two types of nodes:

- **Observed** (triangles): We can measure these variables
- **Latent** (circles): Hidden, unobserved variables



The Causal Markov Condition

How do causal structures constrain probability distributions?

Causal Markov Condition

A probability distribution $P(X_1, \dots, X_n)$ is **classically compatible** with a DAG iff it factorizes as:

$$P(x_1, \dots, x_n) = \prod_{i=1}^n P(x_i \mid \text{parents}(X_i)).$$

Interpretation: Each variable is independent of its indirect causes and non-causes (non-descendants) given its direct causes (parents).

Simple Example

For Clouds \rightarrow Rain \rightarrow Traffic:

$$P(\text{clouds, rain, traffic}) = P(\text{clouds}) \cdot P(\text{rain} \mid \text{clouds}) \cdot P(\text{traffic} \mid \text{rain}).$$

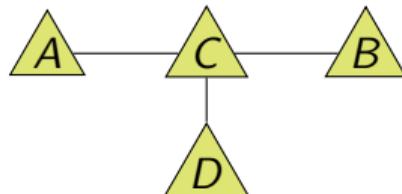
d-separation: Reading Off Independencies

The DAG structure tells us which variables are independent!

d-separation

A graphical criterion to determine conditional independencies from the DAG structure alone.

Example:



Independencies:

- $A \perp B \mid C$
(Given C , A and B are independent)
- $A \perp D \mid C$
- But $A \not\perp B$ unconditionally

Key insight: The graph structure determines which correlations are possible.

Classical vs. Quantum: What's the Difference?

Different theories allow different types of correlations!

Classical Theory:

- Latent nodes = random variables
- Observed nodes = random variables
- Joint distribution satisfies Causal Markov condition
- Set of allowed distributions: \mathcal{C}

Quantum Theory:

- Latent nodes = quantum states
- Observed nodes = quantum measurements (POVMs)
- Joint distribution obtainable from the Born Rule
- Set of allowed distributions: \mathcal{Q}

The hierarchy of the possible sets of distributions

$$\mathcal{C} \subseteq \mathcal{Q} \subseteq \mathcal{G} \subseteq \mathcal{I}$$

where \mathcal{G} = set of correlations obtainable in any Generalised Probabilistic Theory, \mathcal{I} = set of correlations satisfying only the observed conditional independences (weakest constraints).

Classical vs. Quantum in arbitrary causal structures

Central Question

For which causal structures is $\mathcal{C} \subsetneq \mathcal{Q}$? (Classical-quantum gap?)

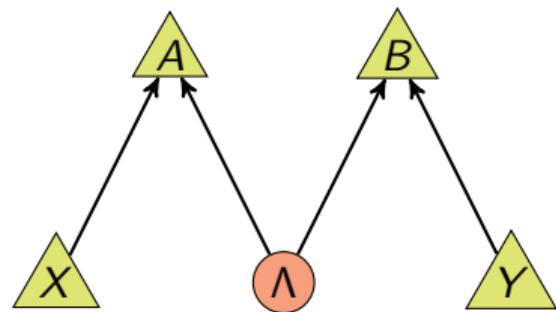
An easier question

For which causal structures is $\mathcal{C} \subset \mathcal{I}$?

Because if $\mathcal{C} = \mathcal{I}$ then trivially $\mathcal{C} = \mathcal{Q}$.

Bell's Theorem: The First Classical-Quantum Gap (C-Q gap)

Bell (1964): Quantum mechanics violates Local Causality (under the assumption of measurement independence)



Classical factorization:

$$P(a, b, x, y) = \sum_{\lambda} Q(a|x, \lambda)Q(b|y, \lambda)Q(x)Q(y)Q(\lambda).$$

This is **local causality**.

Figure: The Bell DAG

Bell's Result

Classical distributions (where sources are hidden variables) satisfying this must obey Bell inequalities. But quantum mechanics can violate them! Hence $\mathcal{C} \subsetneq \mathcal{Q}$ for the Bell DAG.

What are Classical and Quantum distributions in the Bell Causal Structure: An example for sets \mathcal{C} and \mathcal{Q}

The set of Classically compatible distributions is:

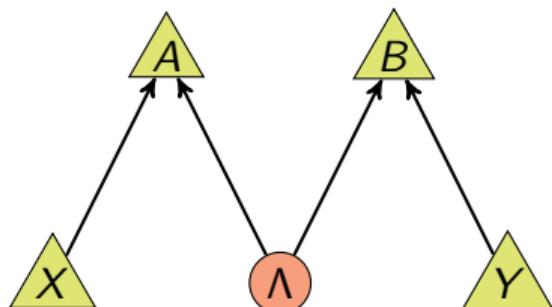


Figure: The Bell DAG

By Bell's theorem $\mathcal{C} \subset \mathcal{Q}$ and therefore there is a Classical-Quantum gap in the Bell DAG.

$$\mathcal{C} = \left\{ P(a, b, x, y) : P(a, b, x, y) = \sum_{\lambda} Q(a | x, \lambda) Q(b | y, \lambda) Q(x) Q(y) Q(\lambda) \right\}$$

The set of Quantum Mechanically compatible distributions is:

$$\mathcal{C} = \left\{ P(a, b, x, y) : P(a, b, x, y) = \text{Tr} (\rho_{AB} E_x^A \otimes E_y^B) P(x)P(y) \right\}$$

Beyond Bell: Which Other Structures Have a C-Q Gap?

Are there other causal structures with classical-quantum gaps?

- **Fritz (2012):** Triangle scenario has a gap
- **HLP (2014):** Classified 366,565 causal structures with ≤ 6 nodes
 - Showed $366,565 - 21$ (*modulo redundancies*) structures have **no C-Q gap**
 - Left 21 candidates that *could* have a C-Q gap

Prior to this work

Known gaps: Bell, Instrumental, Triangle, Unrelated Confounders (*special names given to certain causal structures*)

Progress: Following the technique of Fritz, 16 more shown by Fox et al. (upcoming)

Remaining: Only 1 open case for ≤ 6 nodes (our focus!)

Our Contribution

We resolve the last open case, completing the classification for all causal structures with ≤ 6 nodes!

The Remaining Open Case: G1

Causal structure G1:

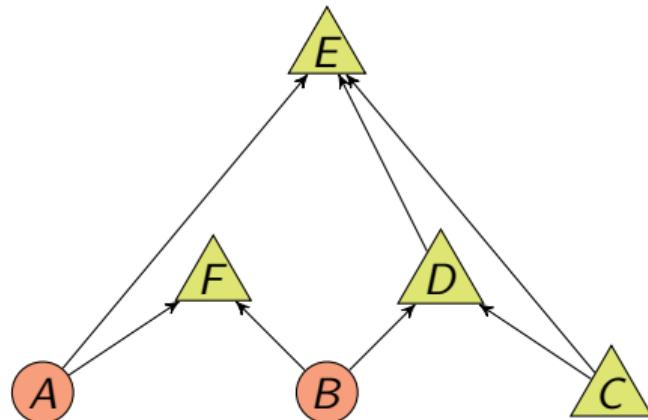


Figure: The causal structure G_1 that is the focus of this work.

Challenge:

- 2 latent nodes: A, B
- 4 observed nodes: C, D, E, F
- Complex connectivity
- Standard techniques don't work

Question:

Does G_1 support quantum correlations that cannot be realized classically?

Our Main Theorem

Yes! There exist quantum correlations compatible with G_1 that have no classical explanation within G_1 .

Our Strategy: Imposing Additional Conditions

Key insight: Consider a restricted subset of correlations

Additional Conditions

- ① **Variable splitting:** Let $F = (F_O, F_S)$ where $F_S = E$ always
- ② **Independence:** Let E be independent of C and D in the observed distribution, i.e., $P(e|cd) = P(e)$

What do these conditions achieve?

- Force E to be determined entirely by A (not influenced by C or D)
- Effectively “turn off” the causal links $C \rightarrow E$ and $D \rightarrow E$
- Make E independent of B (**the most important part**)
- Create a Bell-like structure hidden within G1!

Strategy

- ① Show: Classical + Conditions 1,2 \Rightarrow Bell's local causality
- ② Construct: Quantum correlations violating this (using entanglement)

Classical Compatibility with G1

What does it mean for correlations to be classically compatible with G1?

Definition: Classical Compatibility

$P(CDEF)$ is classically compatible with G1 if \exists a joint distribution $Q(ABCDEF)$ such that:

$$P(cdef) = \sum_{a,b} Q(abcdef)$$

$$\text{where } Q(abcdef) = Q(a)Q(b)Q(c)Q(d|bc)Q(e|acd)Q(f|ab)$$

Interpretation:

- Each term $Q(x_i|\text{parents}(X_i))$ reflects direct causal influence
- Marginalization over latent variables A, B gives observed distribution

Quantum Compatibility with G1

In the quantum case, latent nodes are quantum states

Definition: Quantum Compatibility

$P(CDEF)$ is quantum mechanically compatible with G1 if there exist:

- Hilbert spaces $H_A^E, H_A^F, H_B^F, H_B^D$
- Quantum states ρ_A on $H_A^E \otimes H_A^F$ and ρ_B on $H_B^F \otimes H_B^D$
- POVMs (measurements):
 - $\{K_d^c\}_d$ on H_B^D (for each c)
 - $\{M_e^{c,d}\}_e$ on H_A^E (for each c, d)
 - $\{N_f\}_f$ on $H_A^F \otimes H_B^F$

such that:

$$P(cdef) = \text{tr} \left((M_e^{c,d} \otimes N_f \otimes K_d^c)(\rho_A \otimes \rho_B) \right) P(c)$$

Key: Node B can hold an entangled state!

Lemma 1: Classical Case Reduces to Bell Scenario

With our additional conditions, classical correlations must satisfy Bell's local causality form

Lemma 1 (Classical + Conditions \Rightarrow Local Causality)

If $P(CDEF)$ is classically compatible with G1 and satisfies Conditions 1 and 2, then:

$$P(cdef_O) = \sum_b Q(b)Q(c)Q(e)Q(d|bc)Q(f_O|be).$$

Key observations:

- This is exactly Bell's local causality form!
- "Settings": E (determined by A) and C
- "Outcomes": F_O and D
- Shared common cause: B

Proof approach:

- ① Start with classical factorization from G1
- ② Apply d-separation relations:
 $F \perp CD|B$, $E \perp B|CD$, $B \perp C$
- ③ Use Conditions 1 and 2 to simplify

Proof Sketch of Lemma 1 (Part 1)

Step 1: Start with classical compatibility

$$\begin{aligned} P(cdef) &= \sum_{a,b} Q(abcdef) \\ &= \sum_{a,b} Q(b)Q(c|b)Q(d|bc)Q(e|bcd)Q(f|bcde)Q(a|bcdef) \end{aligned}$$

Step 2: Apply d-separation relations from Theorem 1:

- $F \perp CD|B \Rightarrow Q(f|bcd) = Q(f|b)$
- $E \perp B|CD \Rightarrow Q(e|bcd) = Q(e|cd)$
- $B \perp C \Rightarrow Q(c|b) = Q(c)$

This gives:

$$P(cdef) = \sum_b Q(b)Q(c)Q(d|bc)Q(e|cd)Q(f|bcde)$$

Proof Sketch of Lemma 1 (Part 2)

Step 3: Apply Condition 2: $P(e|cd) = P(e)$

Since $P(e|cd) = \sum_b Q(b)Q(d|bc)Q(e|cd)/(\sum_b Q(b)Q(d|bc))$, we get $Q(e|cd) = Q(e)$

Step 4: Apply Condition 1: $F = (F_O, F_S)$ with $F_S = E$

Replace f with $f_O f_S$ and sum over f_S :

$$P(cdef_O) = \sum_{b, f_S} Q(b)Q(c)Q(d|bc)Q(e)Q(f_O f_S|bcde)$$

Step 5: Simplify using $F_S = E$, $F = (F_S, F_O) = (E, F_O)$

Since $Q(ef_O|bcd) = Q(f_O f_S|bcd) = Q(f|bcd) = Q(f|b) = Q(e|b)Q(f_O|be) = Q(e)Q(f_O|be)$,
(using $Q(e|bcd) = Q(e)$ and $Q(e|cd) = Q(e) \implies Q(e|b) = Q(e)$) we get:

$$P(cdef_O) = \sum_b Q(b)Q(c)Q(e)Q(d|bc)Q(f_O|be)$$

This is Bell's local causality form!

The CHSH Inequality

Bell's local causality implies testable constraints

CHSH Inequality (Clauser, Horne, Shimony, Holt 1969)

For any distribution of the form $P(ab|xy) = \sum_{\lambda} Q(a|x, \lambda)Q(b|y, \lambda)Q(\lambda)$:

$$P(A = B|00) + P(A = B|01) + P(A = B|10) + P(A \neq B|11) \leq 3$$

In our case:

- Settings: E and C (binary)
- Outcomes: F_O and D (binary)
- If classical + Conditions 1,2 hold, then:

$$P(D = F_O|00) + P(D = F_O|01) + P(D = F_O|10) + P(D \neq F_O|11) \leq 3$$

Strategy: Construct quantum correlations that violate this!

Lemma 2: Quantum Violation

Construction using entanglement:

Define $|\theta\rangle = \cos(\theta)|0\rangle + \sin(\theta)|1\rangle$

- ① A : uniformly random classical bit or $A = \frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|11\rangle\langle 11|$
- ② $\rho_B = |\Psi^+\rangle\langle\Psi^+|$ where $|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ (maximally entangled!)
- ③ C : uniformly random classical bit, i.e., $P(C = 0) = P(C = 1) = 0.5$
- ④ $F_S = A$, and F_O is outcome of measuring H_B^F in basis:
 - $\{|0\rangle, |\pi/2\rangle\}$ if $F_S = 0$
 - $\{|\pi/4\rangle, |3\pi/4\rangle\}$ if $F_S = 1$
- ⑤ D is outcome of measuring H_B^D in basis:
 - $\{|\pi/8\rangle, |5\pi/8\rangle\}$ if $C = 0$
 - $\{|-\pi/8\rangle, |3\pi/8\rangle\}$ if $C = 1$
- ⑥ $E = A = F_S$ by both E and F_S measuring $H_A^E, H_A^{F_S}$ in the computational basis $\{|0\rangle, |1\rangle\}$

Result: Standard CHSH calculation gives:

$$P(D = F_O|00) + P(D = F_O|01) + P(D = F_O|10) + P(D \neq F_O|11) = 4 \cos^2(\pi/8) \approx 3.41$$

Obtained distribution violates CHSH! \Rightarrow Classically infeasible in G1

The Probability Distribution

c	e	f_O	d	$P(cef d)$
0	0	0	0	$\frac{1}{8} \cos^2(\pi/8) \approx 0.116$
0	0	0	1	$\frac{1}{8} \sin^2(\pi/8) \approx 0.009$
0	0	1	0	$\frac{1}{8} \sin^2(\pi/8) \approx 0.009$
0	0	1	1	$\frac{1}{8} \cos^2(\pi/8) \approx 0.116$
0	1	0	0	$\frac{1}{8} \cos^2(\pi/8) \approx 0.116$
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1	1	1	0	$\frac{1}{8} \cos^2(\pi/8) \approx 0.116$
1	1	1	1	$\frac{1}{8} \sin^2(\pi/8) \approx 0.009$

Table: Quantum correlations for G1 violating the corresponding CHSH inequality (omitting f_S since $f_S = e$).

Summary of Main Result

Theorem (Main Result)

There exist quantum correlations compatible with G1 that cannot be realized classically in G1.

Proof strategy:

- ① Impose additional conditions that:
 - Isolate a Bell-like substructure
 - Don't necessarily use all causal links
- ② Show classical + conditions \Rightarrow Bell local causality (Lemma 1)
- ③ Construct quantum correlations using entanglement that violate CHSH (Lemma 2)
- ④ Conclude: These quantum correlations have no classical explanation in G1

Application of our strategy

Our method of imposing additional conditions to reveal hidden Bell structures works beyond G1!

Application to G2

Causal structure G2:

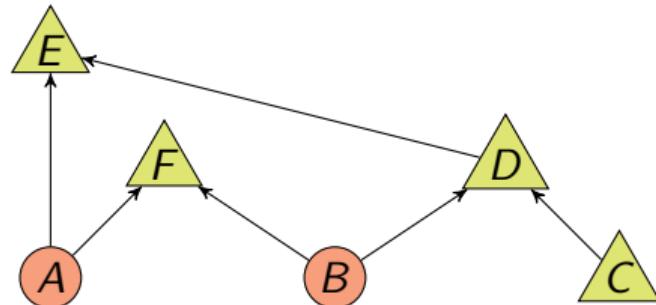


Figure: $G1 = G2$ without $C \rightarrow E$

Immediate corollary:

- Our quantum construction for G1 didn't use the link $C \rightarrow E$
- These same correlations work for G2
- Removing an edge adds constraints
- Hence, the classical set for $G2 \subset$ classical set for G1

Result

G2 also has a classical-quantum gap!

The Triangle Causal Structure

Triangle structure:

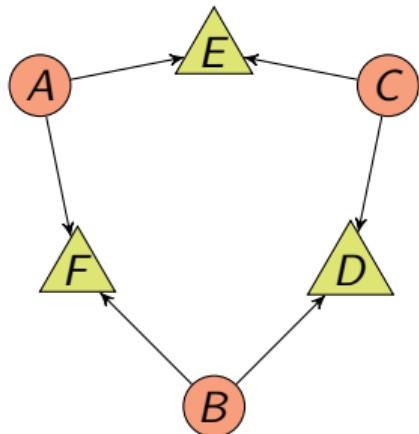


Figure: The triangle causal structure.

Fritz's result (2012):

- Showed that the triangle causal structure has a classical-quantum gap
- Used entropy-based arguments to show this

Our contribution:

- Alternative proof at the level of probabilities using our technique
- More direct construction and easier to follow

Method: Take $D = (S_1, O_1)$, $E = (S'_1, S'_2)$, $F = (S_2, O_2)$ with $S'_1 = S_1$ and $S'_2 = S_2$. Then classical compatibility reduces to Bell local causality!

Generalizing the “Fritz Trick”

Our method extends Fritz's approach:

The General Strategy

- ① Identify potential “settings” and “outcomes” in the causal structure
- ② Impose conditions that:
 - Turn off interfering causal paths. If need be consider perfectly correlated bits.
 - Create independence structure mimicking Bell scenario
 - Force settings to be independent of the latent common cause of the outputs
- ③ Prove: Classical + conditions \Rightarrow local causality form
- ④ Construct: Quantum violations using entanglement

Key insight: Work at the level of probabilities, not entropies

- More direct and easier to follow
- Easier to construct explicit quantum violations
- Generalizes more naturally

The Big Picture: All Structures up to 6 Nodes

The journey to complete classification:

- **Total:** 366,565 causal structures with ≤ 6 nodes
- **HLP (2014):** Ruled out 366,544 (no gap possible or any possible gap can be reduced to the remaining 21)
- **Remaining:** 21 candidates

Resolution of the 21 Cases

Bell (1964):

Bell DAG

Fritz (2012):

Triangle

Instrumental (2018-19):

Instrumental scenario

Unrelated Confounders (2024):

Simplest causal network

Fox et al. (upcoming):

Following the technique of Fritz, 16 more cases out of the 21 remaining

This work (2025):

G1 (the last case!)

Post-Quantum Correlations

Can we go beyond quantum mechanics?

Hierarchy of Correlation Sets

$$\mathcal{C} \subseteq \mathcal{Q} \subseteq \mathcal{G} \subseteq \mathcal{I}$$

- \mathcal{C} : Classical (local hidden variables)
- \mathcal{Q} : Quantum (entanglement, measurements)
- \mathcal{G} : Generalised Probabilistic Theories
- \mathcal{I} : Graph-compatible (respects DAG observed conditional independencies)

Question: Are there structures where $\mathcal{Q} \subsetneq \mathcal{G}$ (post-quantum correlations) such that $\mathcal{C} \subseteq \mathcal{Q}$?

Result from our work

For ≤ 6 nodes: No! Every structure with potential of $\mathcal{Q} \subsetneq \mathcal{G}$ also necessarily has $\mathcal{C} \subsetneq \mathcal{Q}$.
There are no structures with post-quantum but not non-classical quantum correlations.

Why does this matter?

Foundational:

- Deeper understanding of causality at the level of quantum mechanical systems
- Shows quantum non-classicality is not limited to the Bell causal structure
- No post-quantum correlations without non-classical quantum correlations (for ≤ 6 nodes), indicating the same might be true for larger DAGs

Practical:

- Identifying which experiments can demonstrate quantum advantage
- Causal inference with quantum resources
- Quantum cryptography beyond standard settings

Summary

- ① **Resolved the last open case:** Showed G1 has a classical-quantum gap
- ② **New methodology:** Developed a technique of imposing additional conditions to reveal hidden Bell structure in other structures
- ③ **Complete classification:** All causal structures with ≤ 6 nodes now classified
- ④ **Generalized Fritz's approach:** Applied to multiple structures (G1, G2, Triangle)
- ⑤ **No post-quantum without quantum:** Ruled out intermediate theories for ≤ 6 nodes

Future Directions and Applications

- Experimental demonstrations of quantum violations in different structures
- Causal discovery with quantum data
- Quantum network protocols
- Device-independent applications
- Develop systematic algorithms for finding quantum violations
- Explore connections to other areas such as machine learning and causal inference)

For details, please refer:

1) *Chapter 6 in Khanna, S. (2025). Exploring non-classical correlations in causal scenarios (Doctoral dissertation, University of York).*

https://etheses.whiterose.ac.uk/id/eprint/36307/1/PhD_Thesis_Submitted_Version.pdf

2) *Khanna, S., Pusey, M., Colbeck, R. (2025). Closing the problem of which causal structures of up to six total nodes have a classical-quantum gap.*

arXiv preprint arXiv:2512.04058

<https://arxiv.org/pdf/2512.04058>

Thank You!

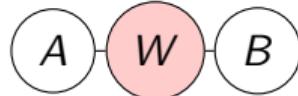
Questions?

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Backup: d-separation in Detail

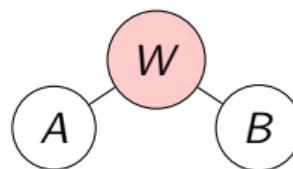
Three types of paths that can be blocked:

Chain:



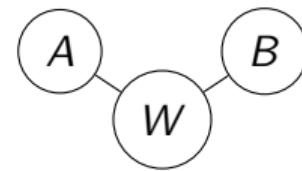
$$A \perp B | W$$

Fork:



$$A \perp B | W$$

Collider:



$A \perp B$ (unconditionally!)
But conditioning on W or
any of its descendants
opens the path

Backup: Full Classical Factorization for G1

Detailed expansion:

Starting from:

$$Q(abcdef) = Q(a)Q(b)Q(c)Q(d|bc)Q(e|acd)Q(f|ab)$$

Expand using conditional probability:

$$\begin{aligned} P(cdef) &= \sum_{a,b} Q(abcdef) \\ &= \sum_{a,b} Q(b)Q(c|b)Q(d|bc)Q(e|bcd)Q(f|bcde)Q(a|bcdef) \end{aligned}$$

Apply d-separations:

- $B \perp C \Rightarrow Q(c|b) = Q(c)$
- $E \perp B|CD \Rightarrow Q(e|bcd) = Q(e|cd)$
- $F \perp CD|B \Rightarrow Q(f|bcd) = Q(f|b)$

Result:

$$P(cdef) = \sum_{a,b} Q(b)Q(c)Q(d|bc)Q(e|cd)Q(f|b)$$