G-RIPS · FUJITSU PROJECT

Topology of Conditional Causality

A Geometric Post-Analysis of Fujitsu's Causal AI

G-RIPS FUJITSU TEAM

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ACKNOWLEDGMENTS

Supported By



Fujitsu ・Tohoku University・MathCCS・Tohoku Forum for Creativity・AIMR・ IPAM ・ National Science Foundation・iTHEMS

BACKGROUND

What is a Causal Graph?





Chocolate eaten

GDP



Nobel prizes

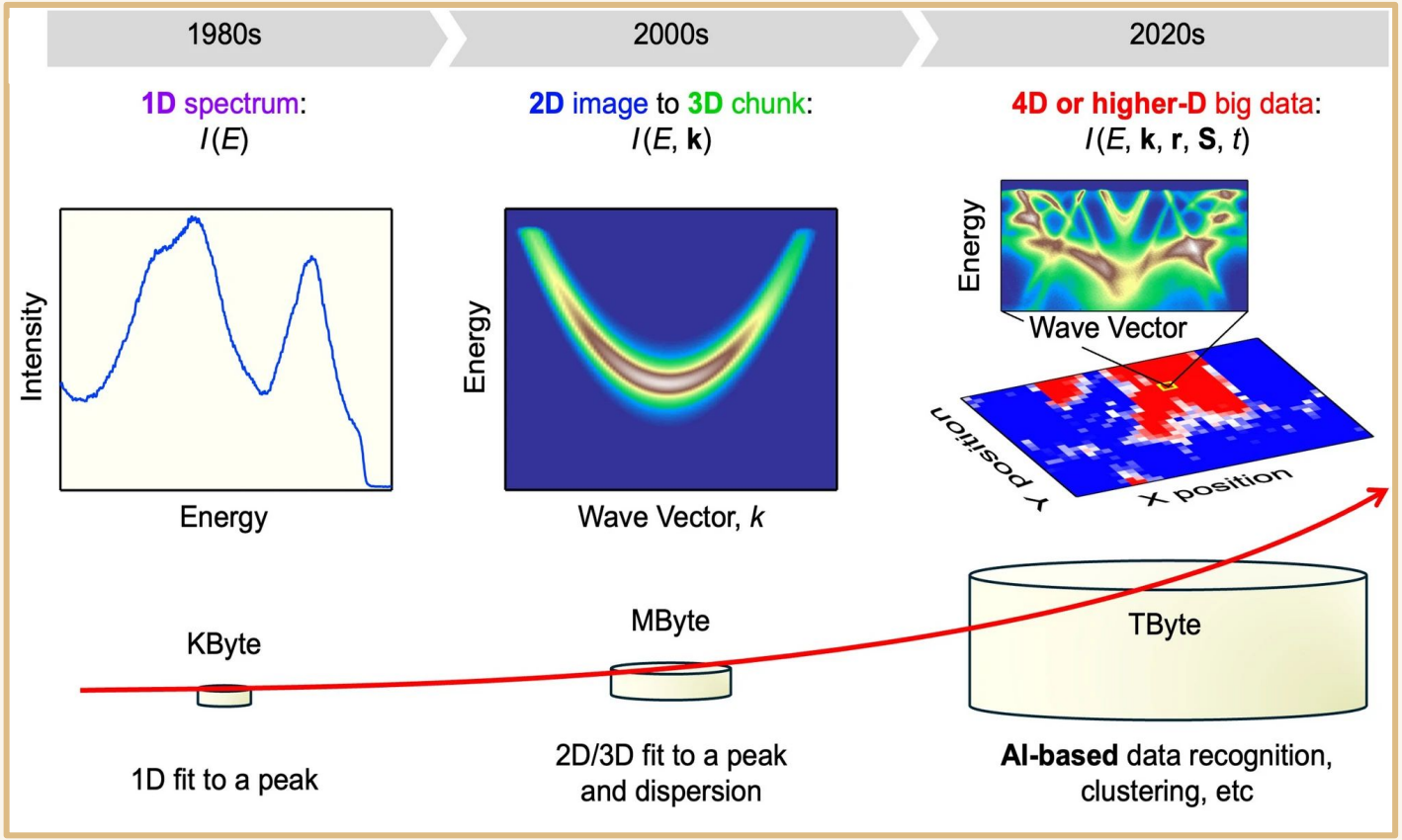
spurious correlation

causality

Ref: F. H. Messerli, N Engl J Med (2012)

Background

Problem : **Data Explosion**
Massive & High-Dimensional Data

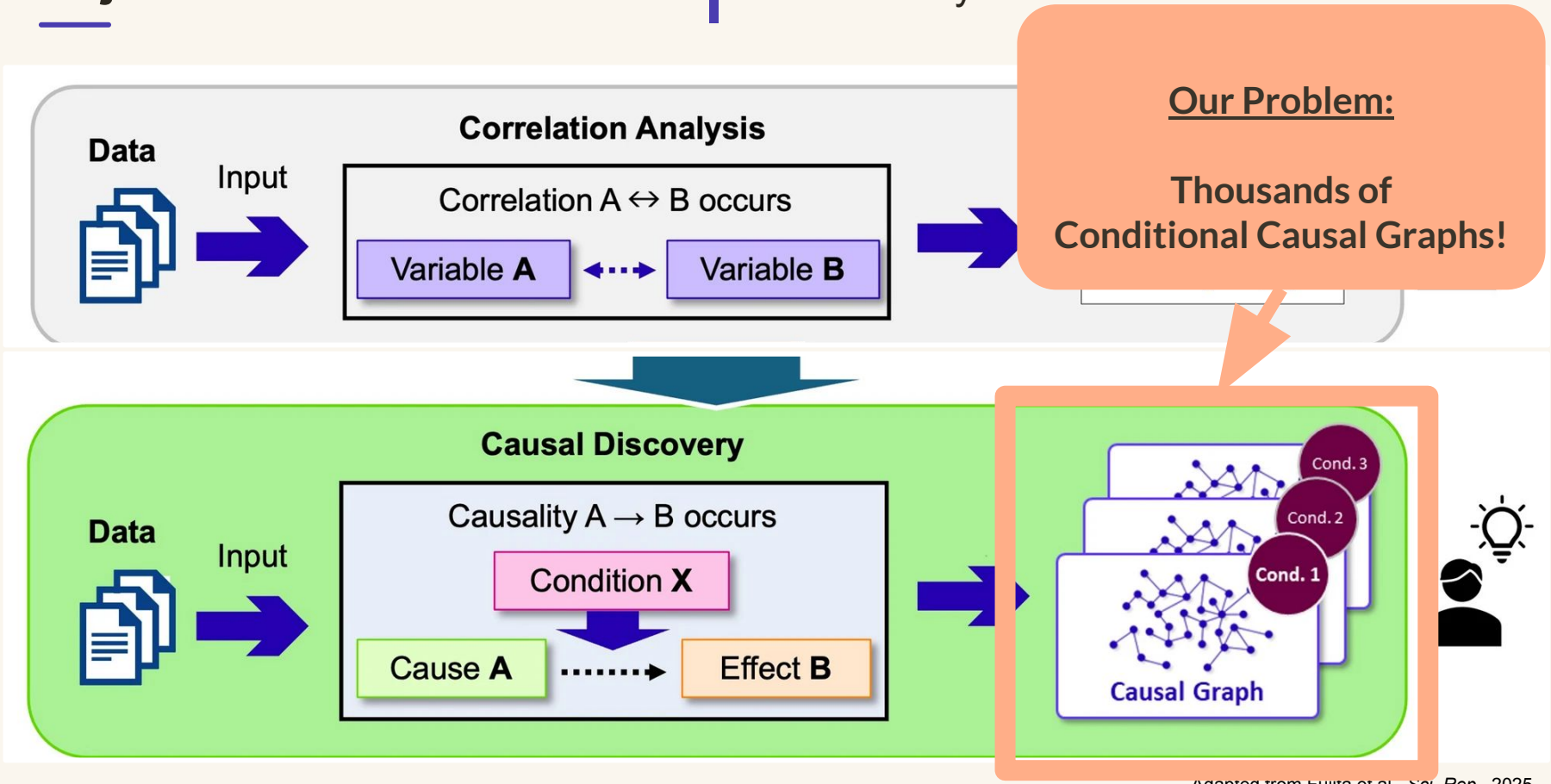


Adapted from Fujita et al., *Sci. Rep.*, 2025

BACKGROUND

Fujitsu Causal AI

Solution : Causal AI
automatically extract causal structures



Adapted from Fujita et al., *Sci. Rep.*, 2025

BACKGROUND

Motivation & Core Objective

Transforming Causal Graphs into Reliable Scientific Insights

Three Pillars for AI-Driven Discovery

1.Convincingness

Logical & Simple

2.Comprehensiveness

Unbiased & Exhaustive

3.Discoverability

Beyond Human Intuition

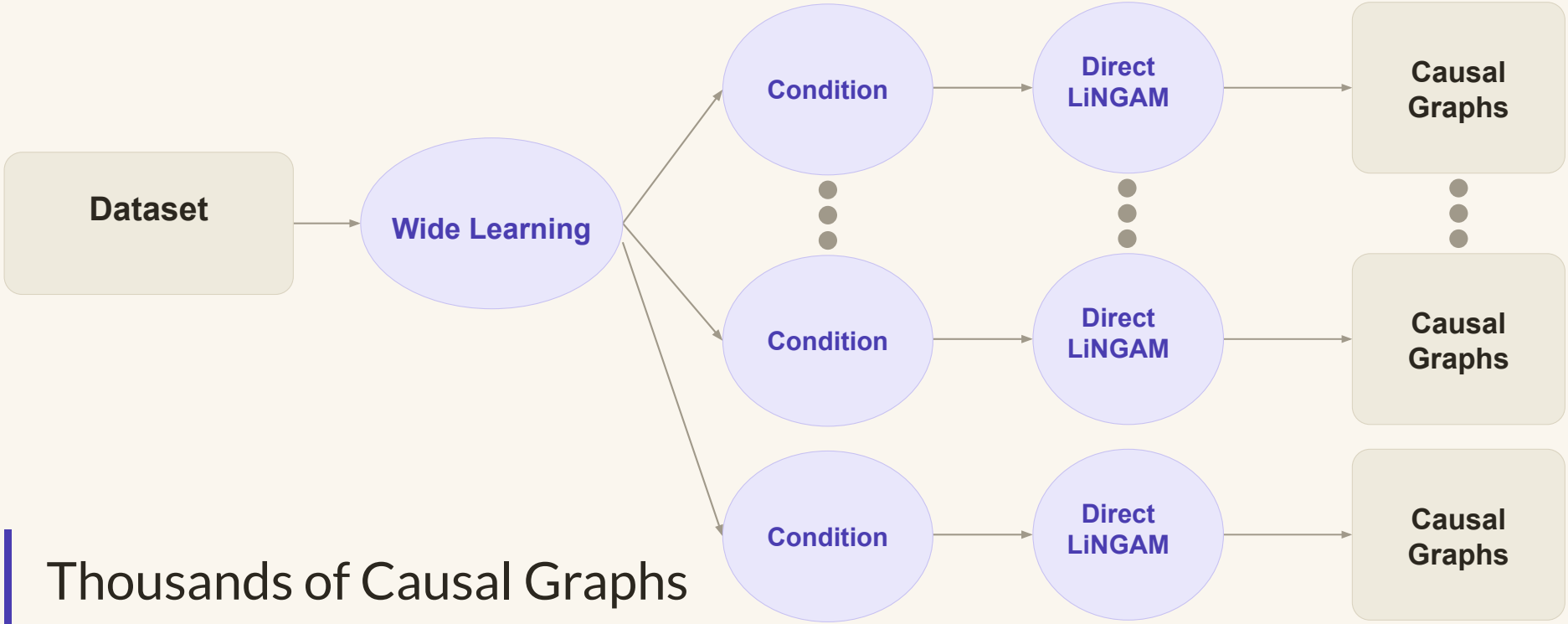
Goal: Enhance Causal AI with a mathematical framework to drive scientific discovery.

BACKGROUND

Inside Fujitsu's Causal AI

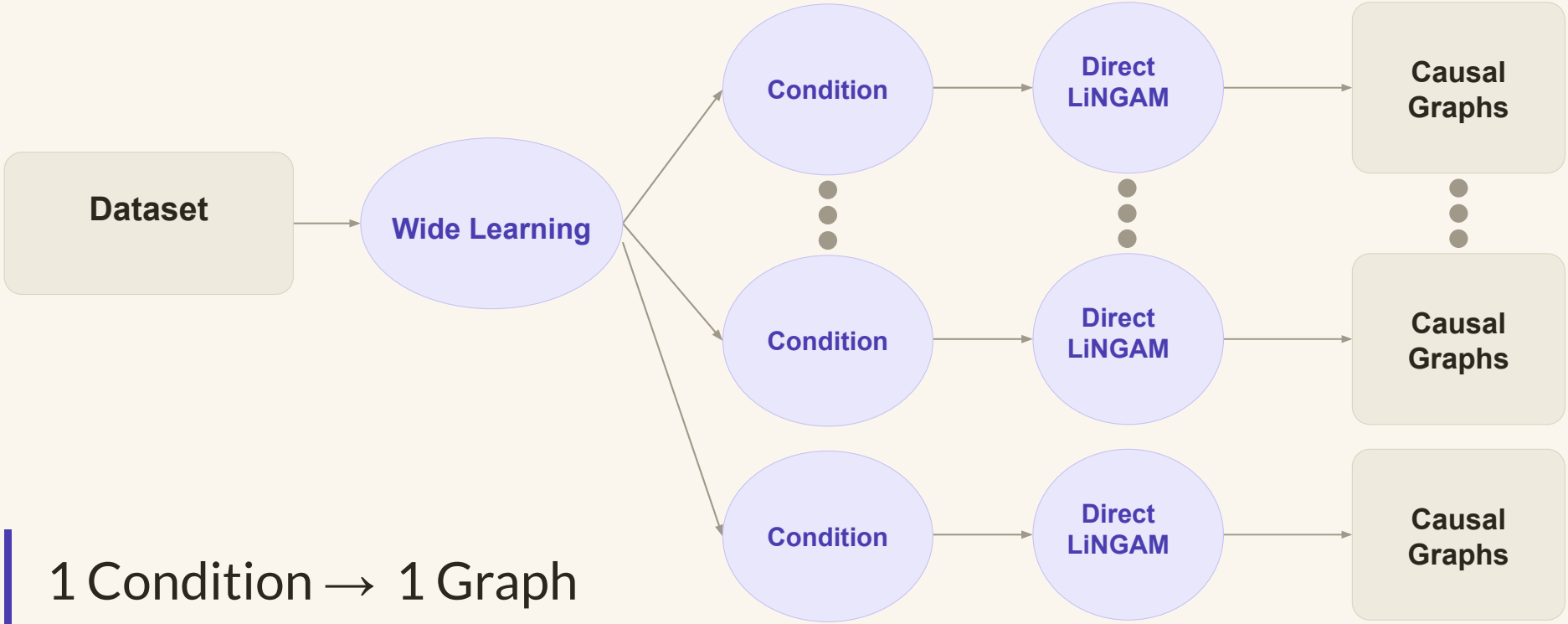


In More Detail



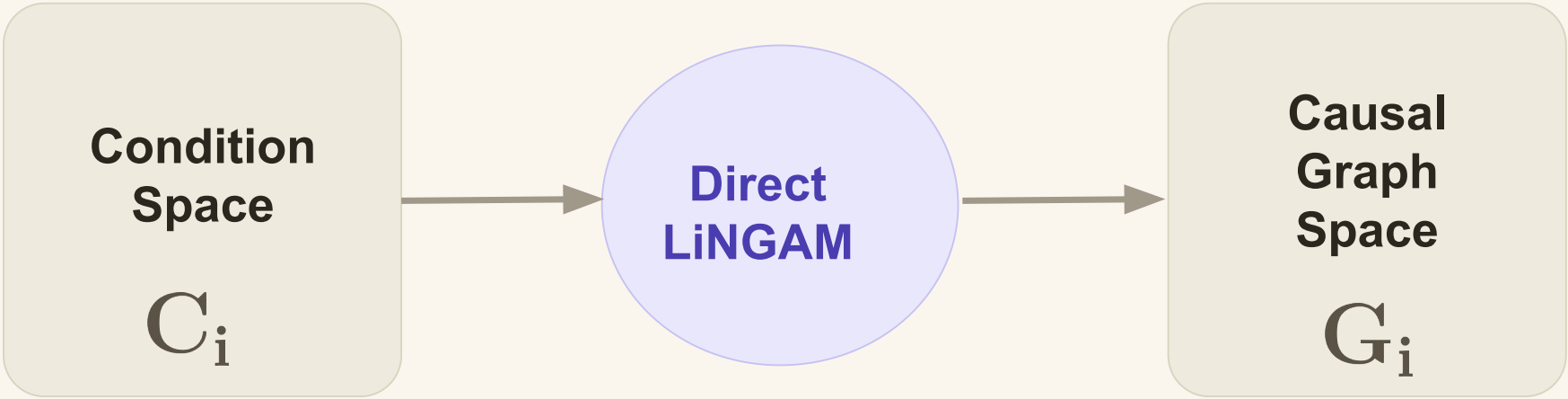
Thousands of Causal Graphs

In More Detail



1 Condition → 1 Graph

Why Use Metrics?



- Goal : analyze (C_i, G_i)
- Need : Metrics

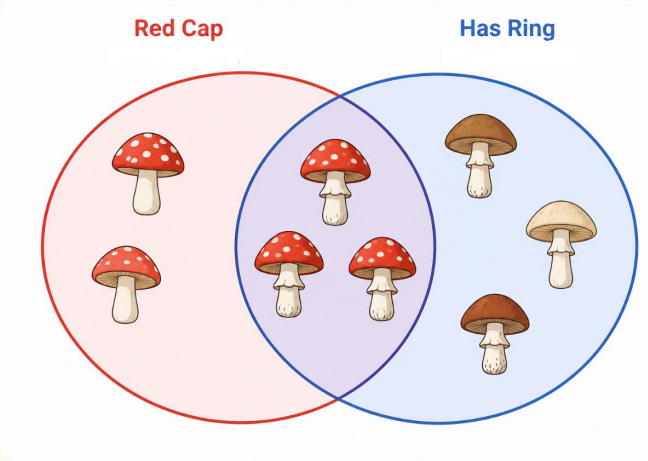
METRICS

A Metric on the Space of Conditions

The Jaccard Metric

How similar two sets are.

$$\mathrm{d_J}(C_1, C_2) = 1 - \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|}$$

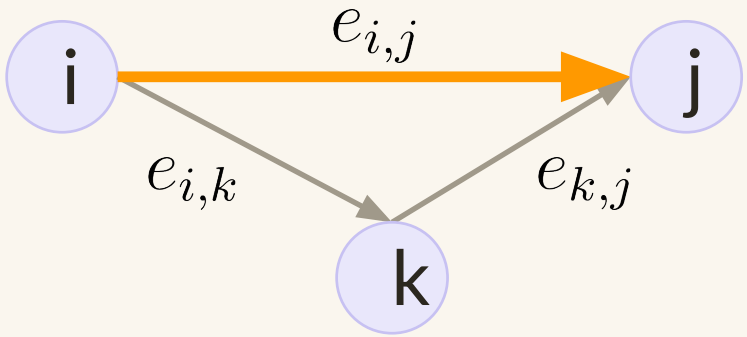


$$\mathrm{d_J}(\mathrm{Red}, \mathrm{Ring}) = 1 - \frac{3}{8} = \frac{5}{8}$$

METRICS

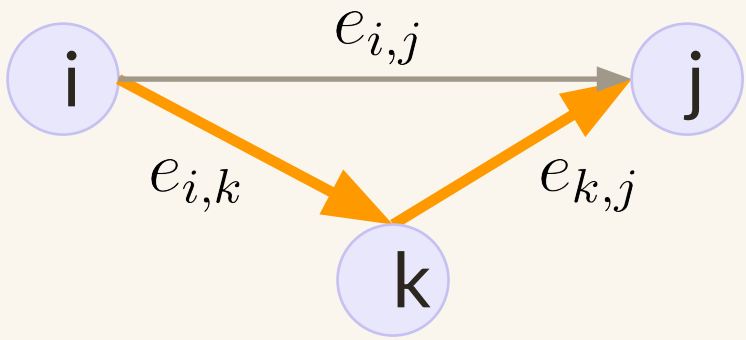
The Total Effect Metric on Causal Graphs

$$\mathbf{R_{i,j} = e_{i,j} + e_{i,k}e_{k,j}}$$



All the ways i cause j

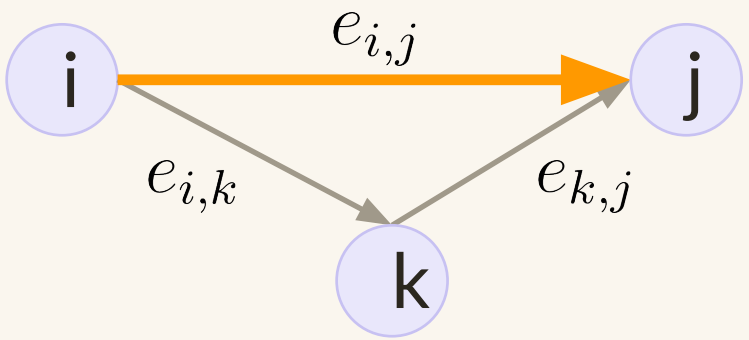
$$\mathbf{d_{TE}(G_1, G_2) = ||R(G_1) - R(G_2)||_F}$$



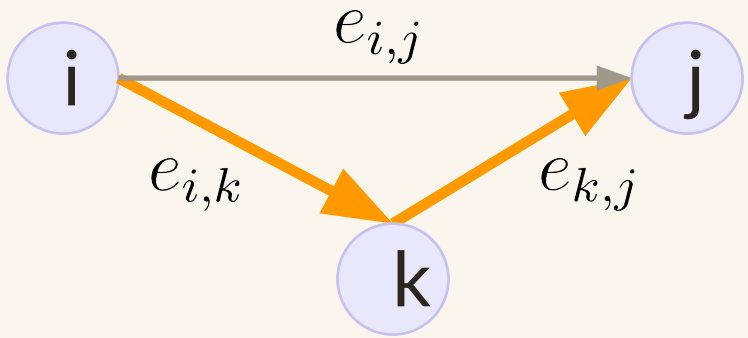
METRICS

Why Total Effect Metric on Causal Graphs

Measures how much influence
i has over j

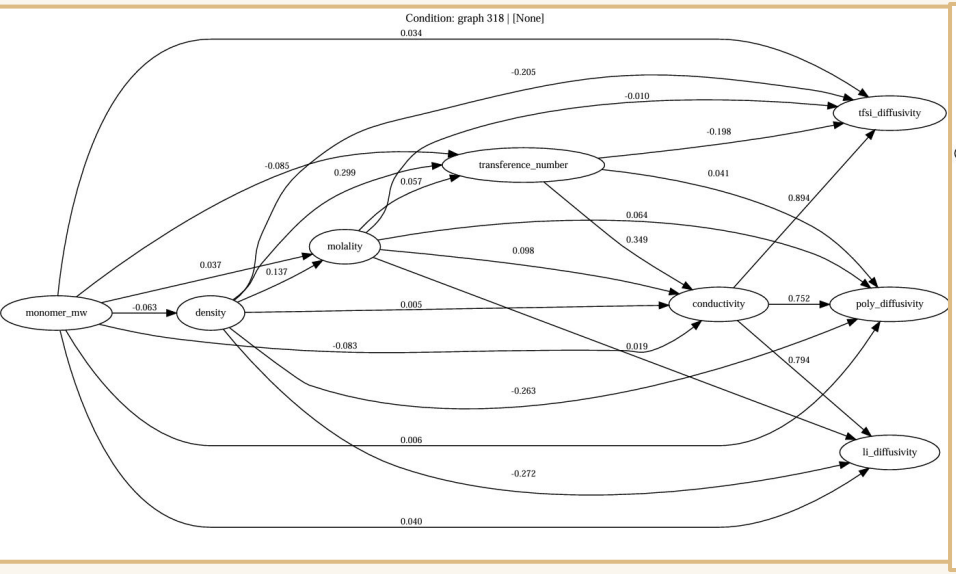


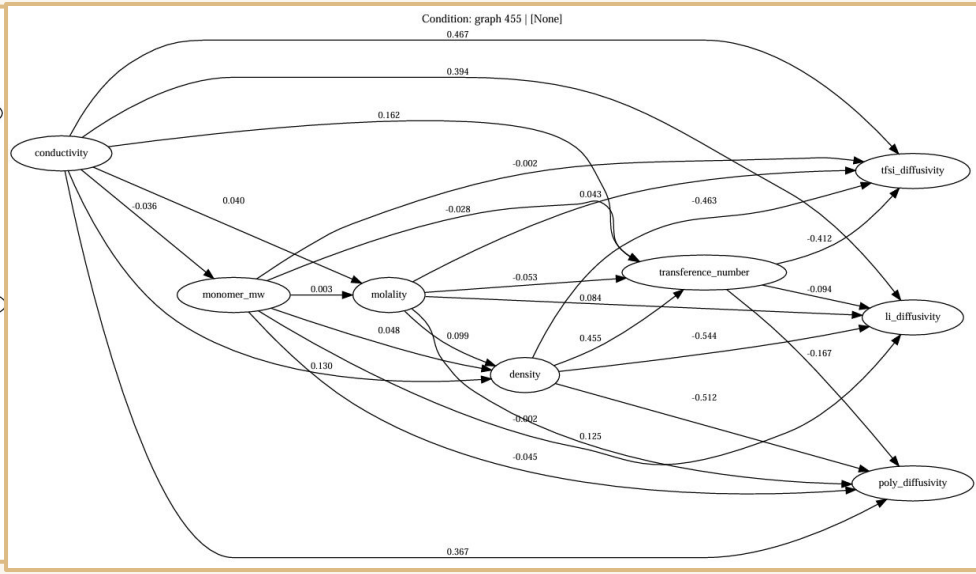
Total Effect matrices provide
comprehensiveness of causality



METRICS

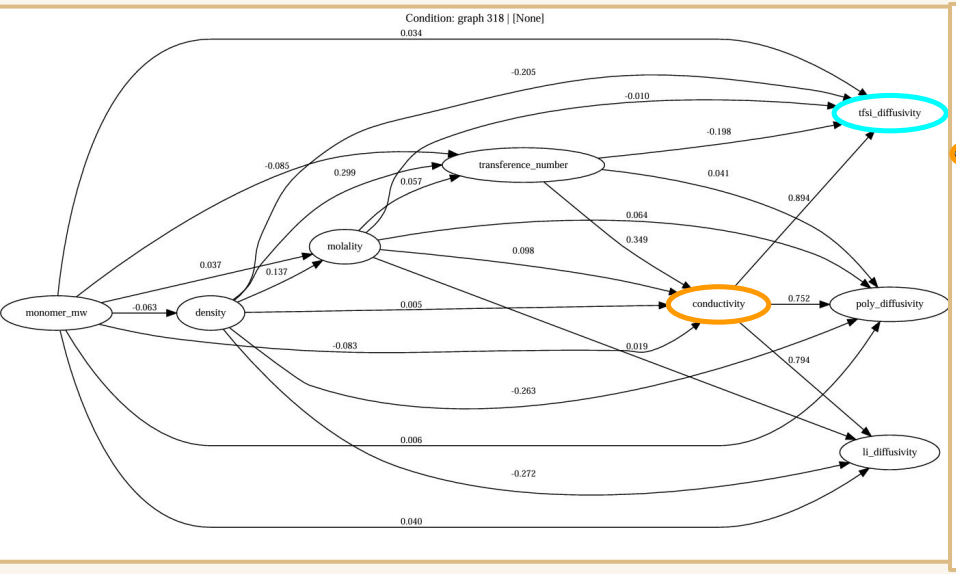
TE and Frobenius metrics

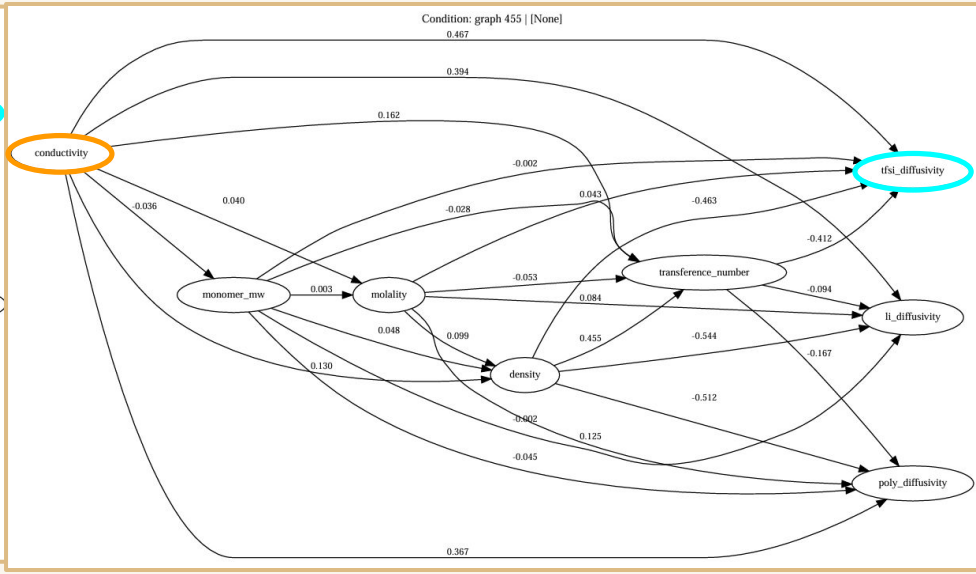




METRICS

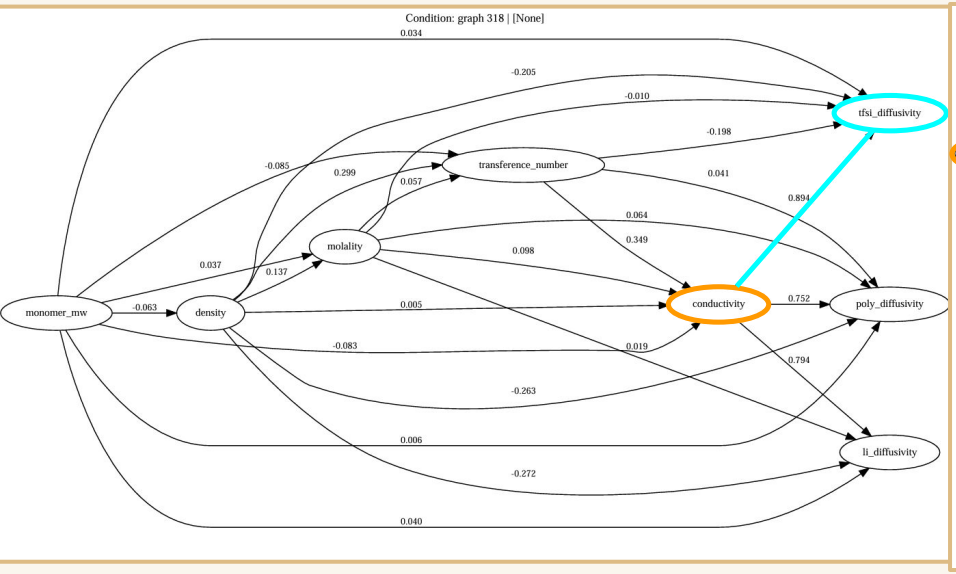
TE and Frobenius metrics

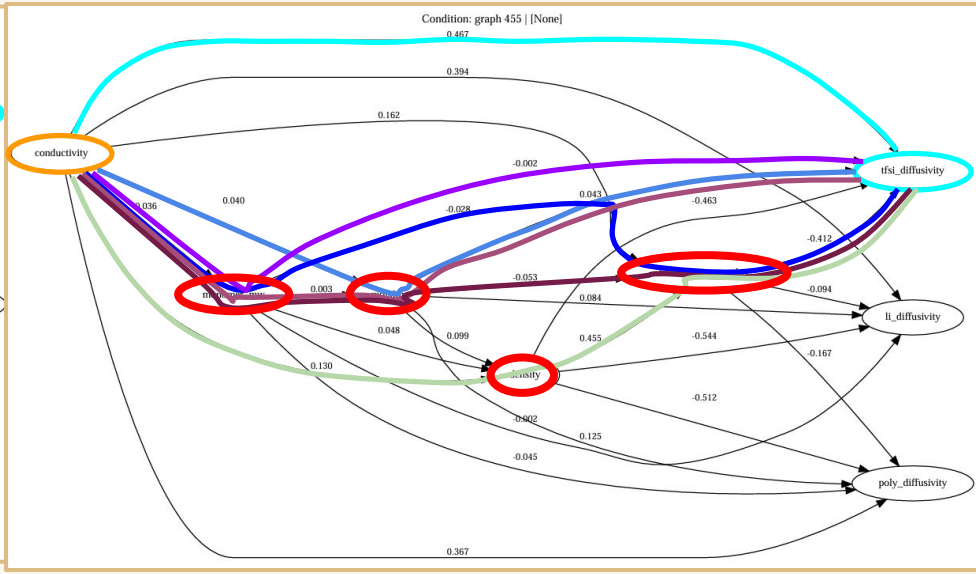




METRICS

TE and Frobenius metrics



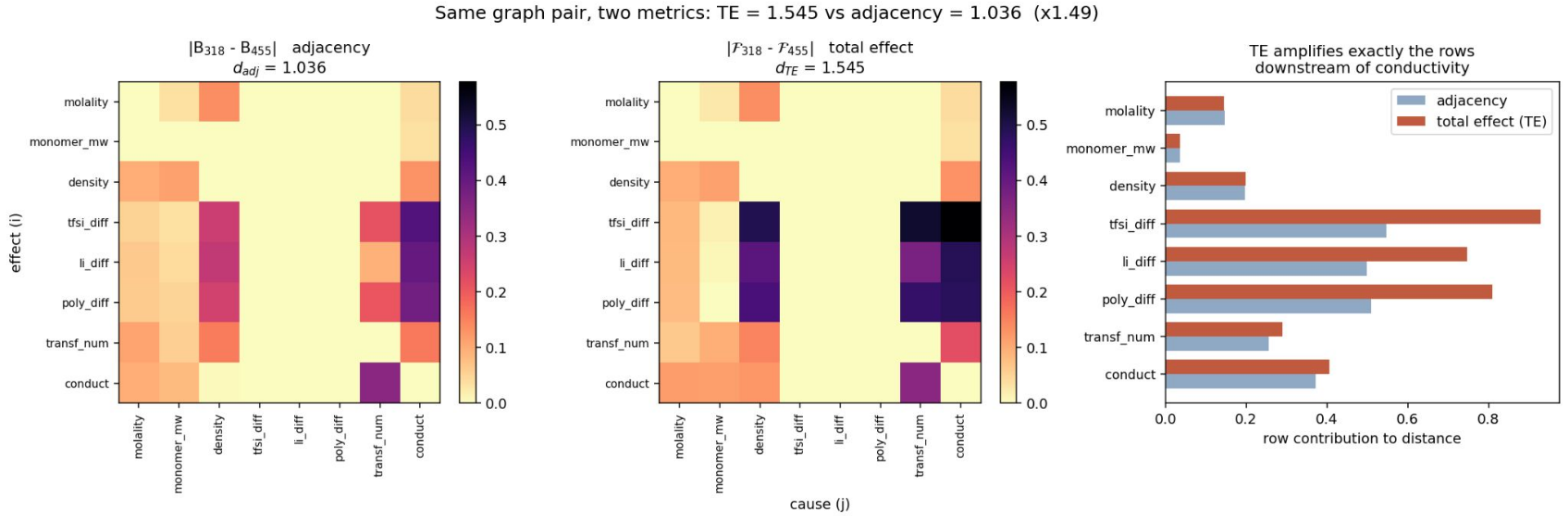


Frobenius : only catch the edges directly connects

Total Effects : collects all the paths

METRICS

TE and Frobenius metrics



The total effect metric shows the accumulation of all paths

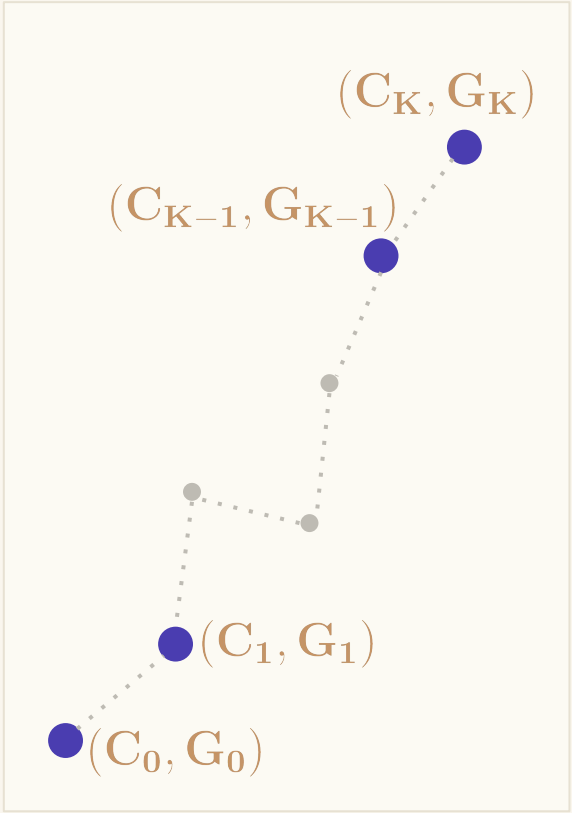
CONDITIONAL PATHING

Path-connecting causal graphs

Path exists:
Type of Conditional homogeneity

Can we find a **path**?

No path exists:
Distinct causal structures



DEFINITION

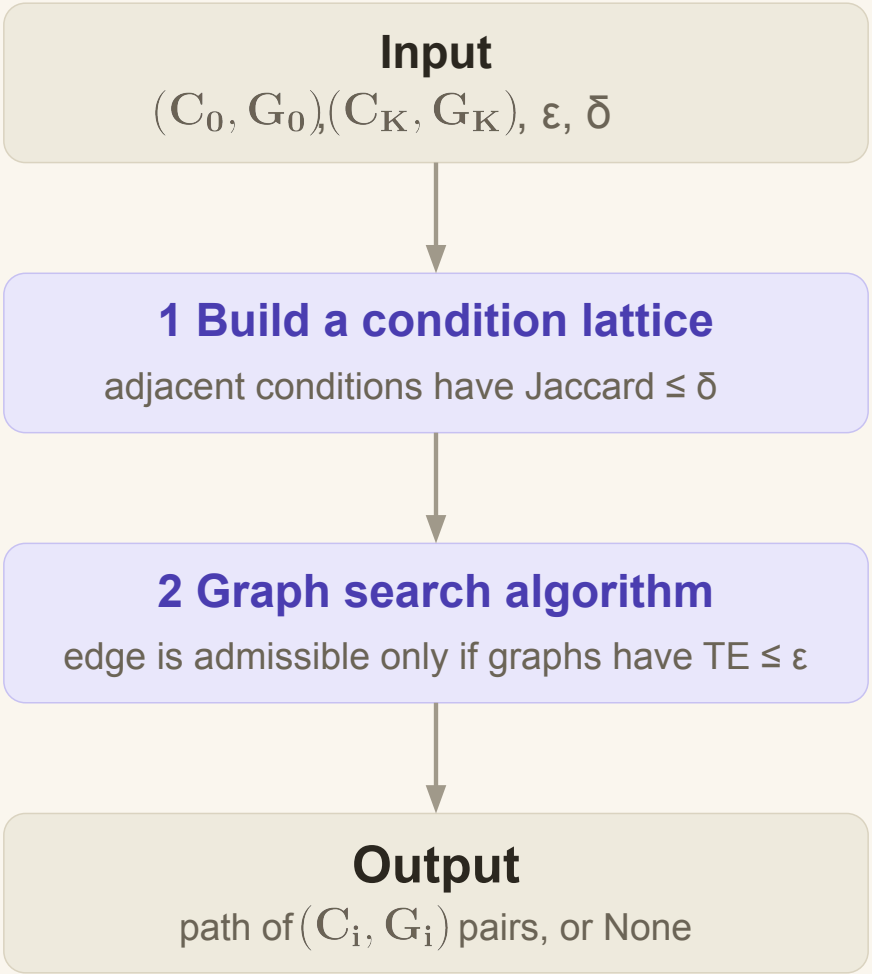
(C_0, G_0) and (C_K, G_K) are **(ε,δ)-path connected** if there exists some $\{C_i\}$ so that at every step,

$$d_{TE}(G_i, G_{i+1}) \leq \epsilon$$

$$d_J(C_i, C_{i+1}) \leq \delta$$

CONDITIONAL PATHING

The pathing algorithm



CONDITIONAL PATHING

The pathing algorithm

Input

$(C_0, G_0), (C_K, G_K)$, ε, δ

1 Build a condition lattice

adjacent conditions have Jaccard ≤ δ

2 Graph search algorithm

edge is admissible only if graphs have TE ≤ ε

Output

path of (C_i, G_i) pairs, or None

Tradeoff!

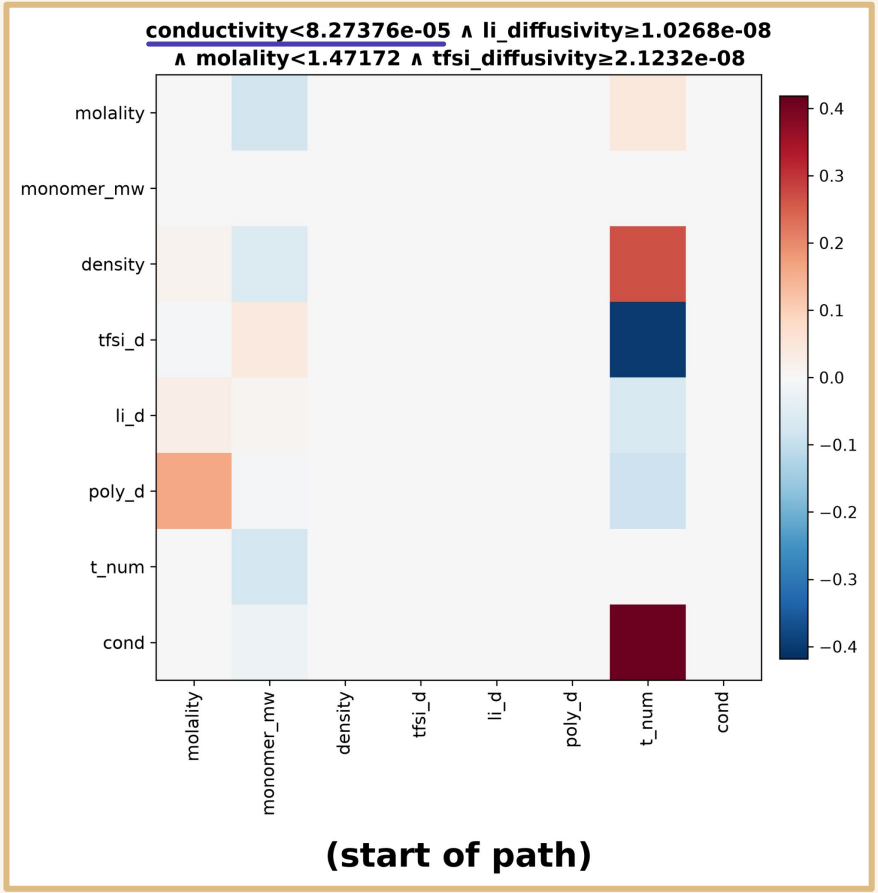
Comprehensiveness



Computational Cost

CONDITIONAL PATHING

The pathing algorithm

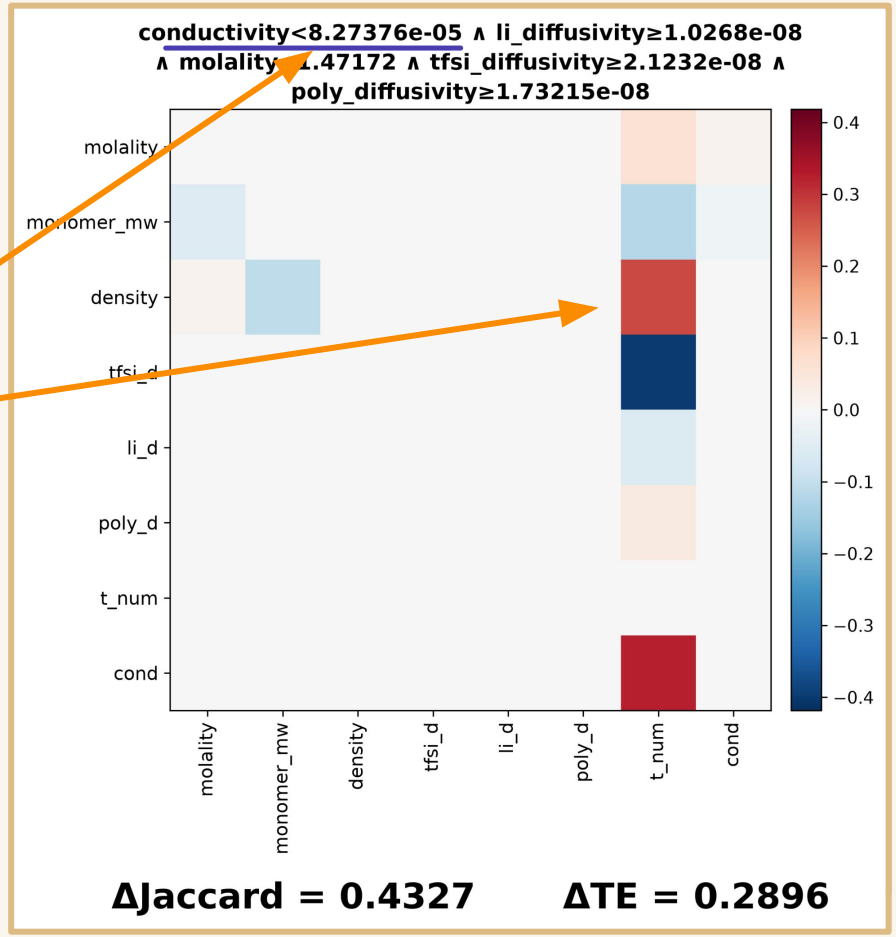


0->1->2->3->4->5->6

CONDITIONAL PATHING

The pathing algorithm

Doesn’t change!

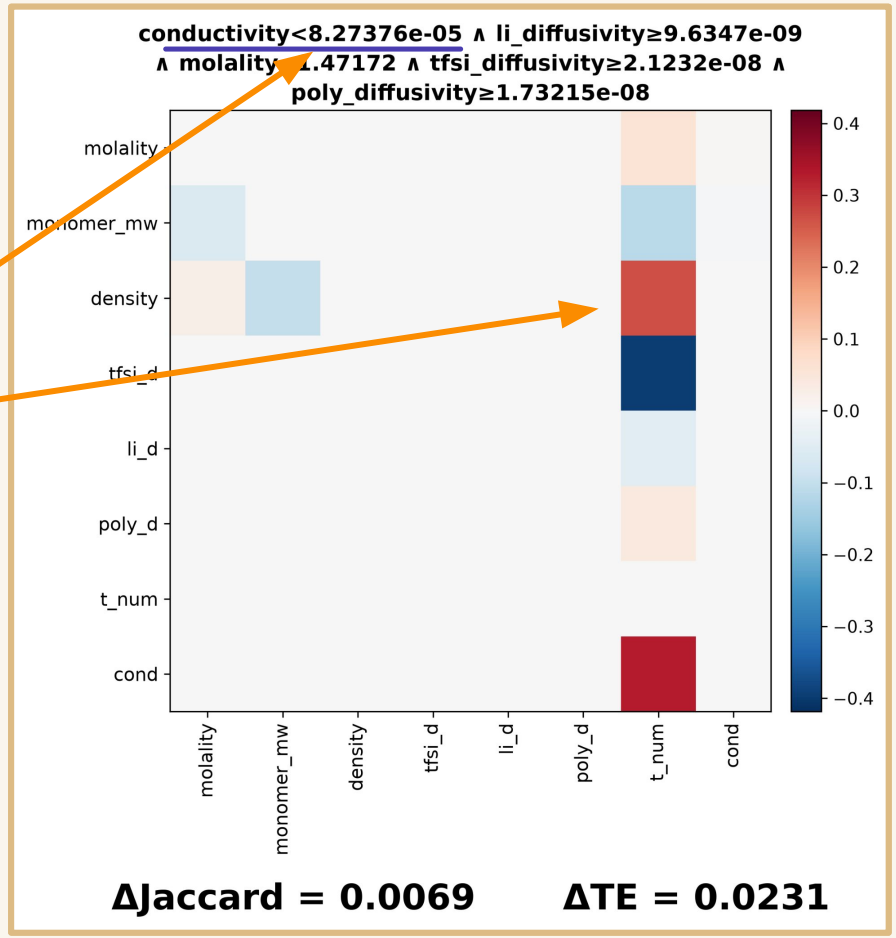


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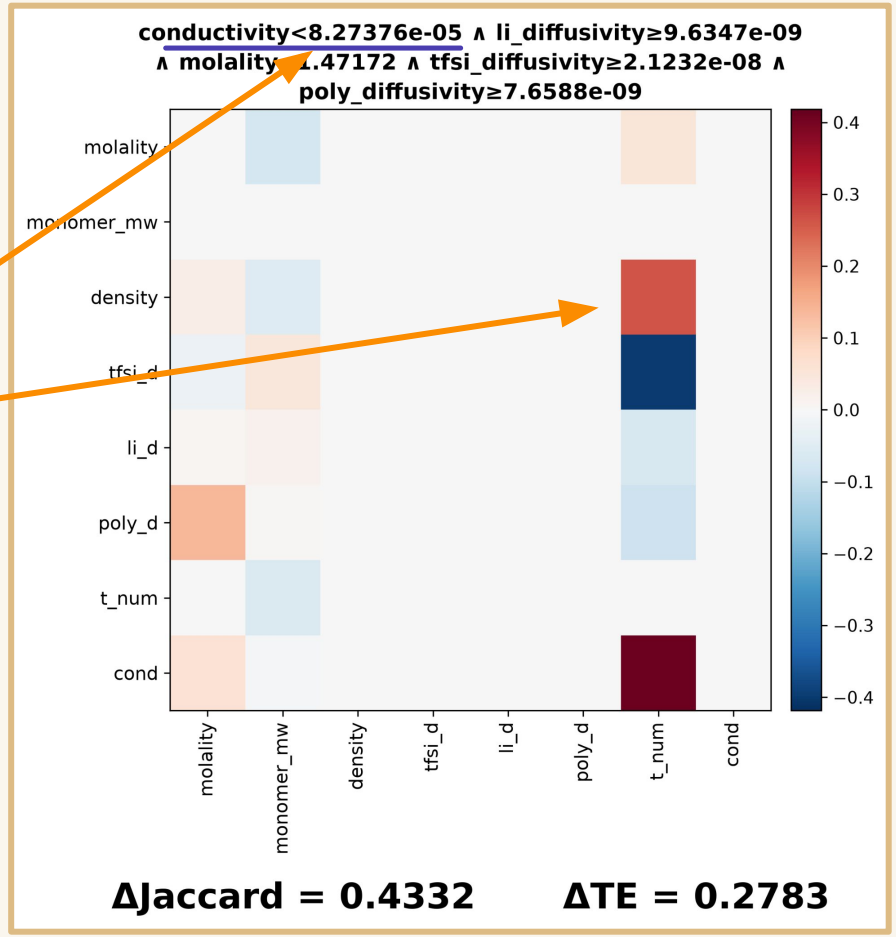


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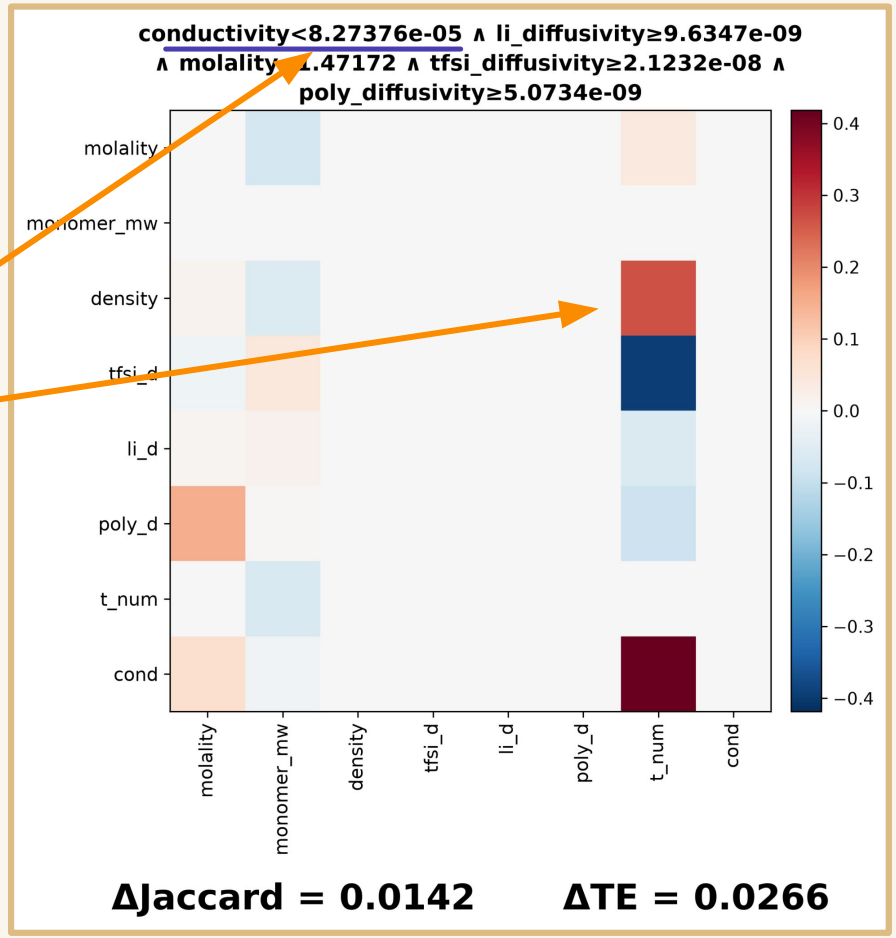


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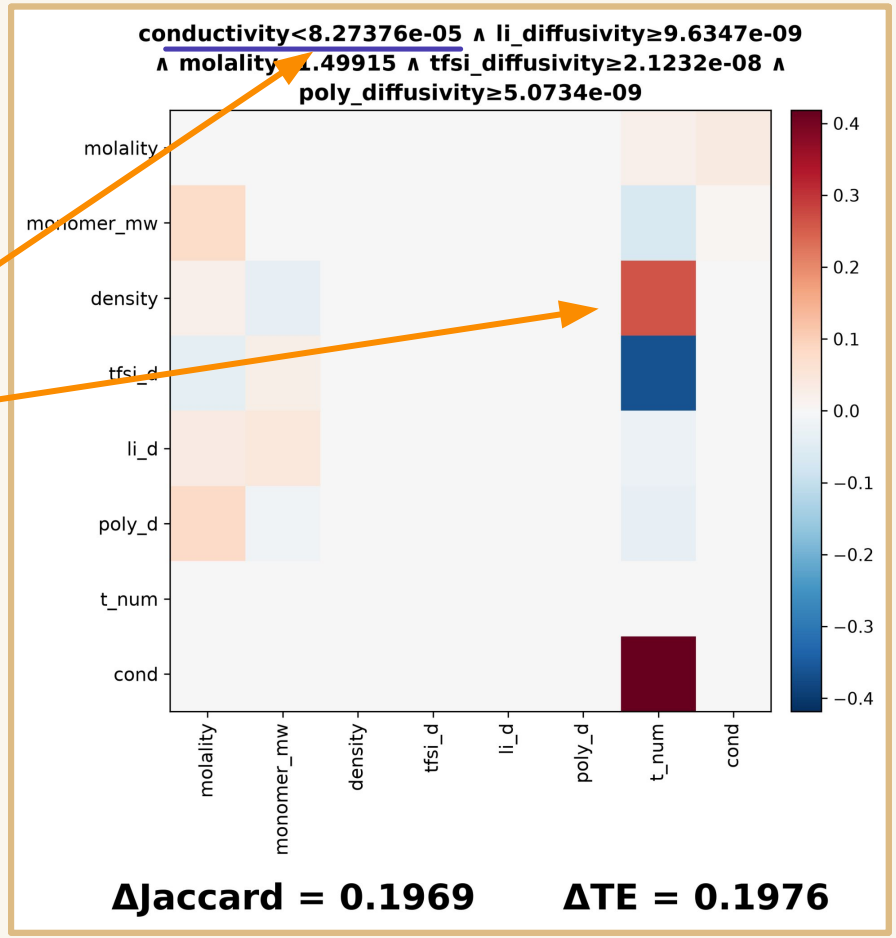


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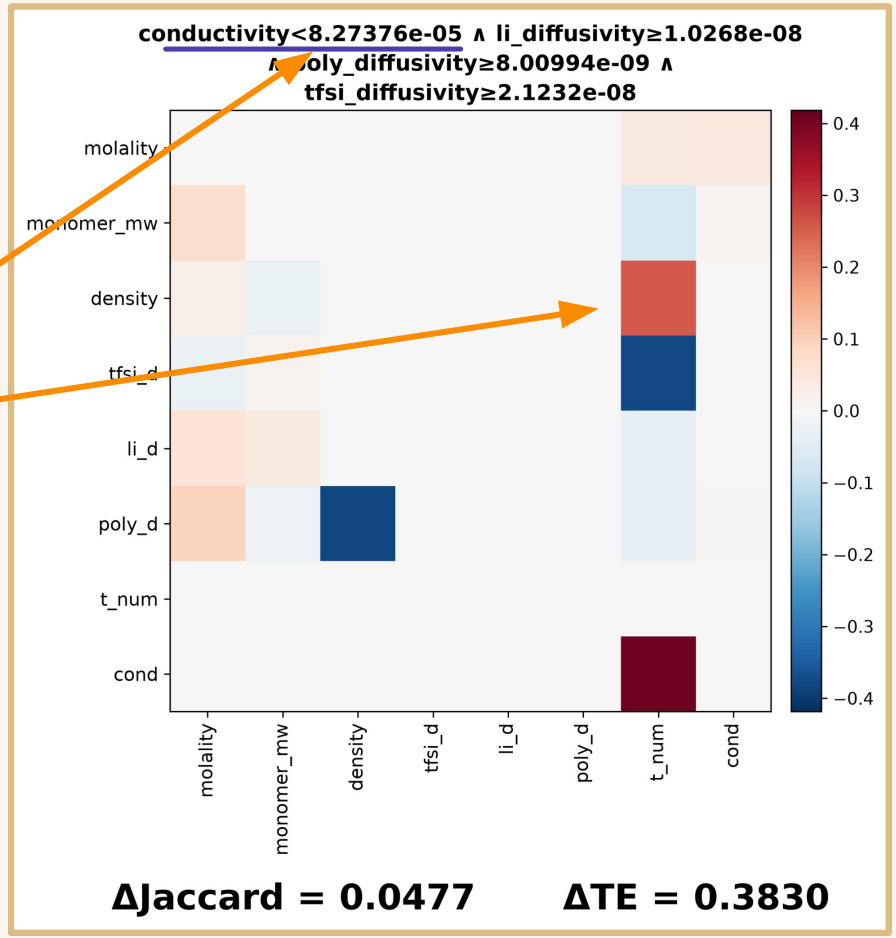


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CONDITIONAL PATHING

The pathing algorithm

Doesn’t change!



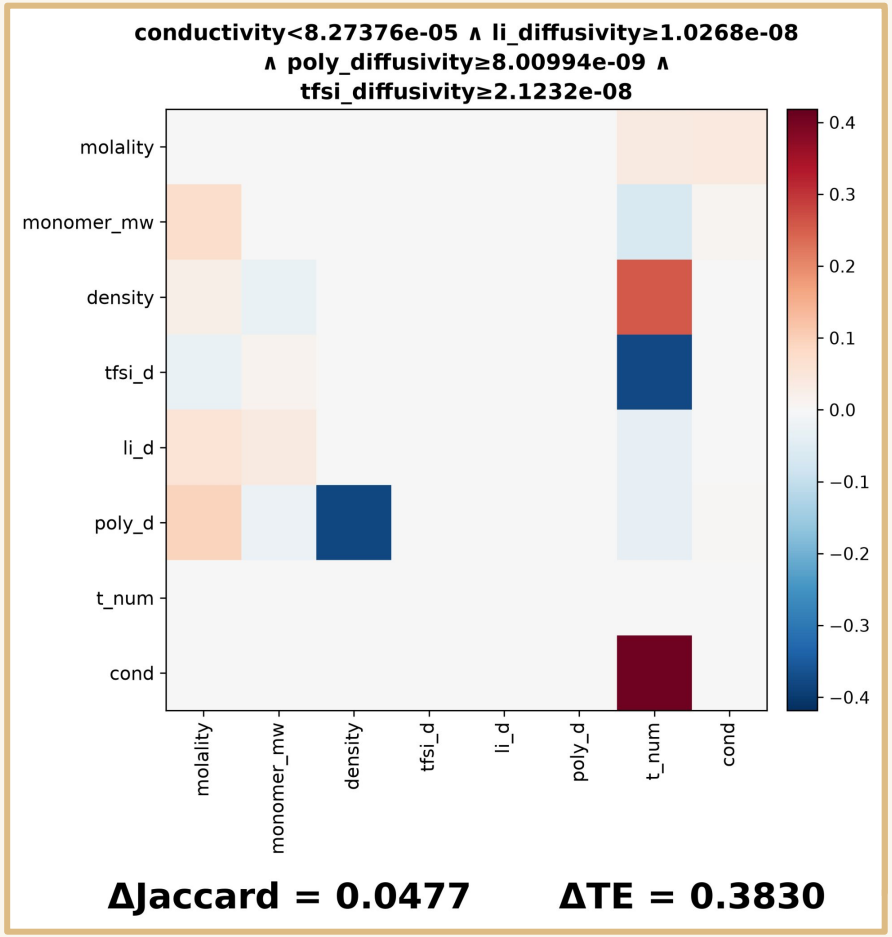
0->1->2->3->4->5->6

CONDITIONAL PATHING

The pathing algorithm

Some conditions are *load bearing candidates* (**conductivity, tfsi_diffusivity**)

Potential **drivers** of a fixed **mechanism**



0->1->2->3->4->5->6

CONDITIONAL PATHING

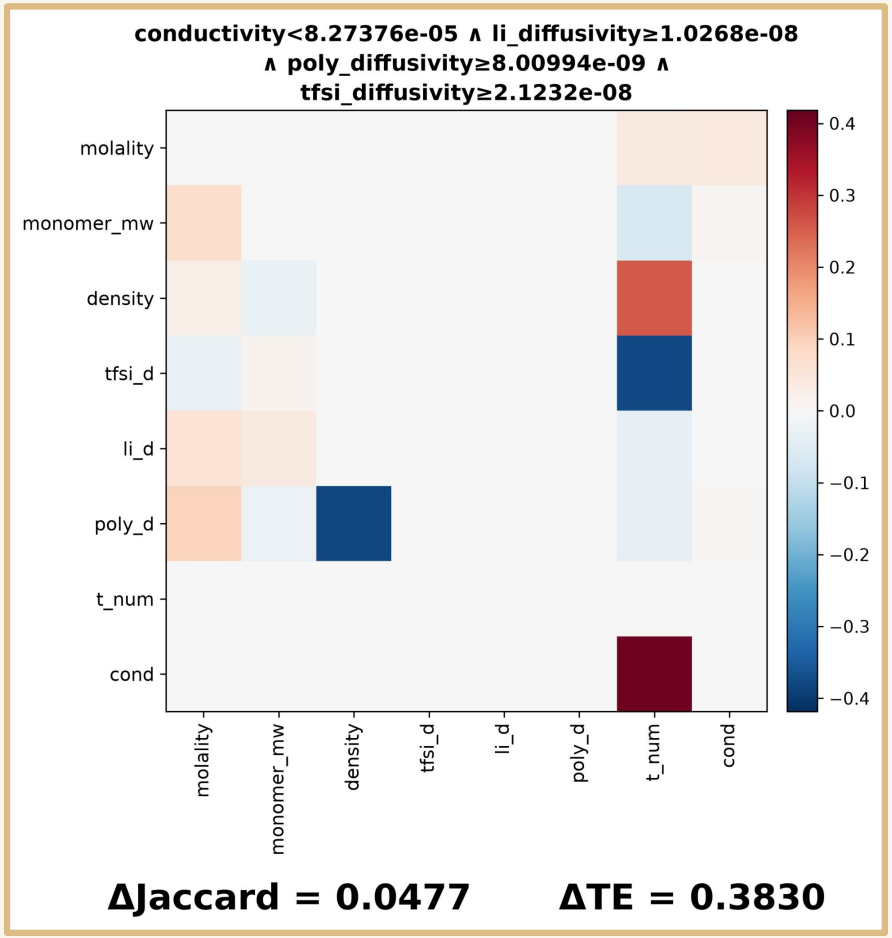
The pathing algorithm

Some conditions are *load bearing candidates* (**conductivity, tfsi_diffusivity**)

Potential **drivers** of a fixed **mechanism**

Structural finding

Not physics



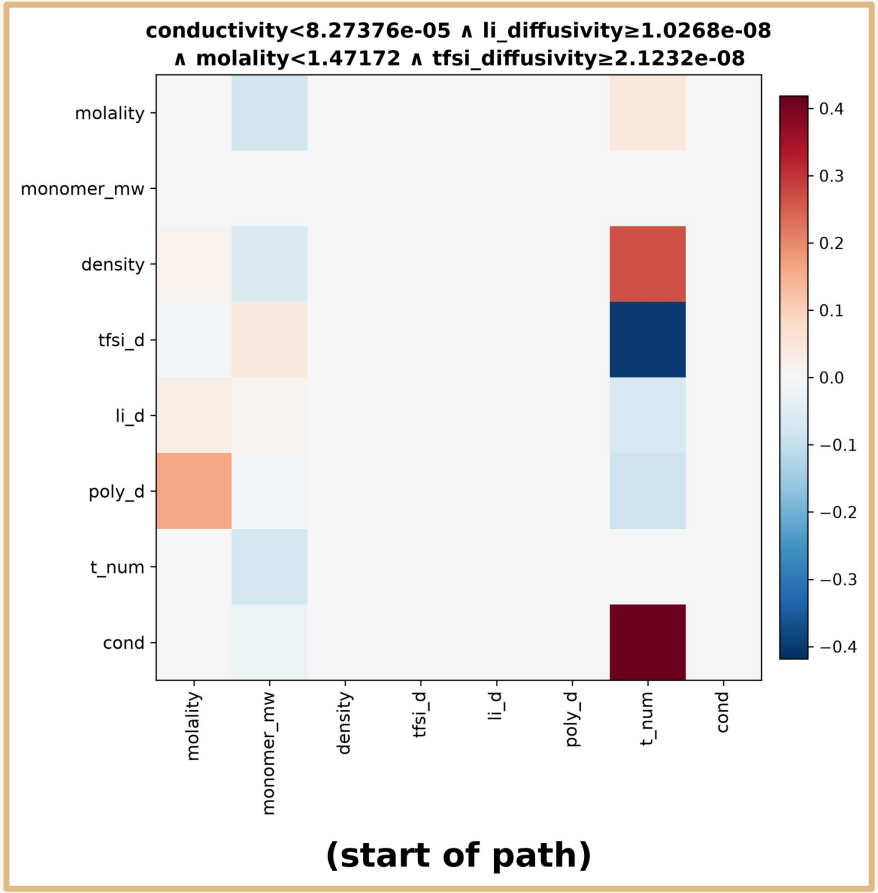
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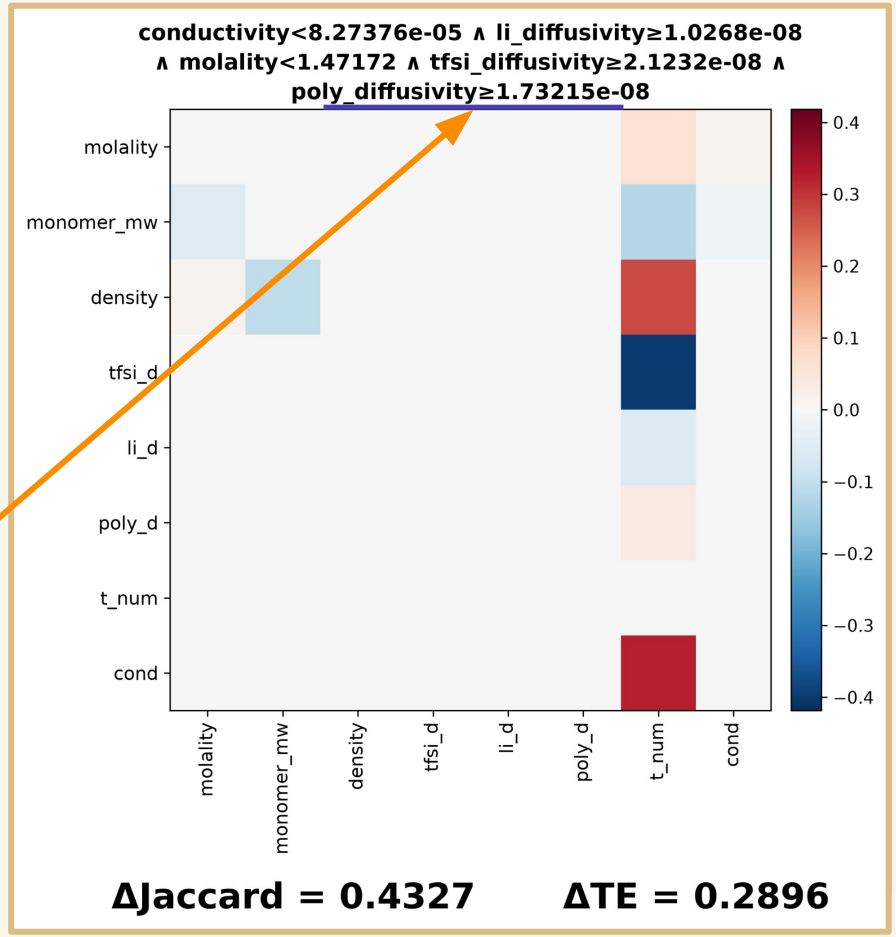
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Changes “freely”!



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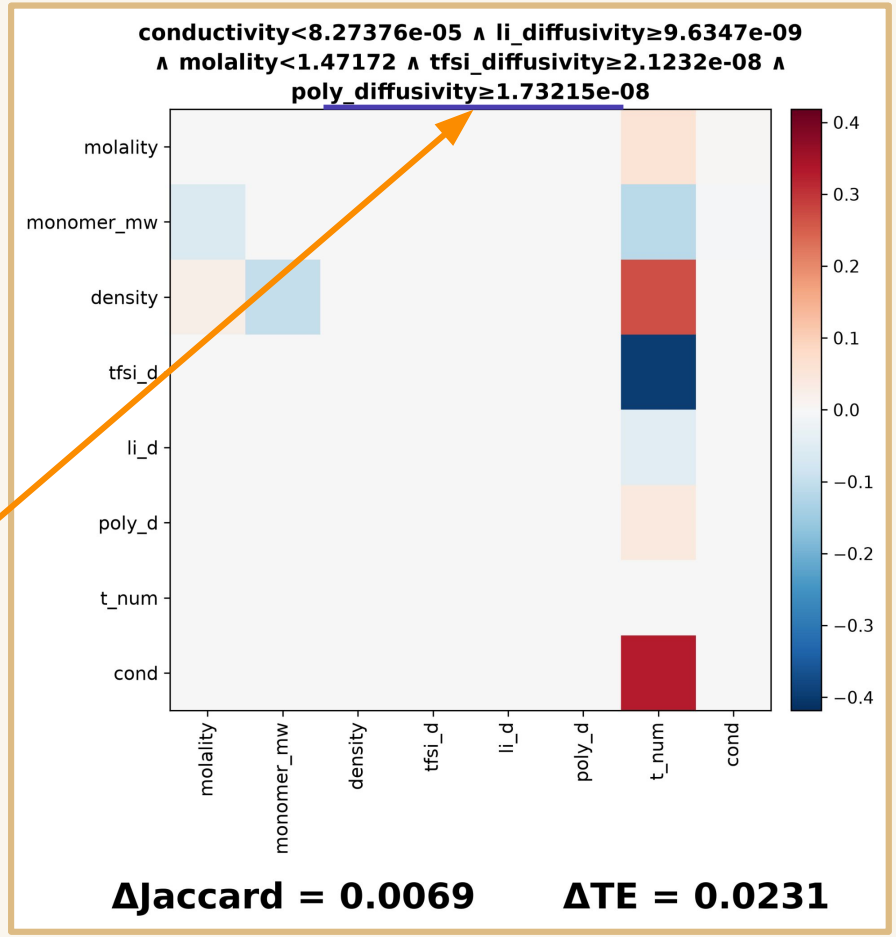
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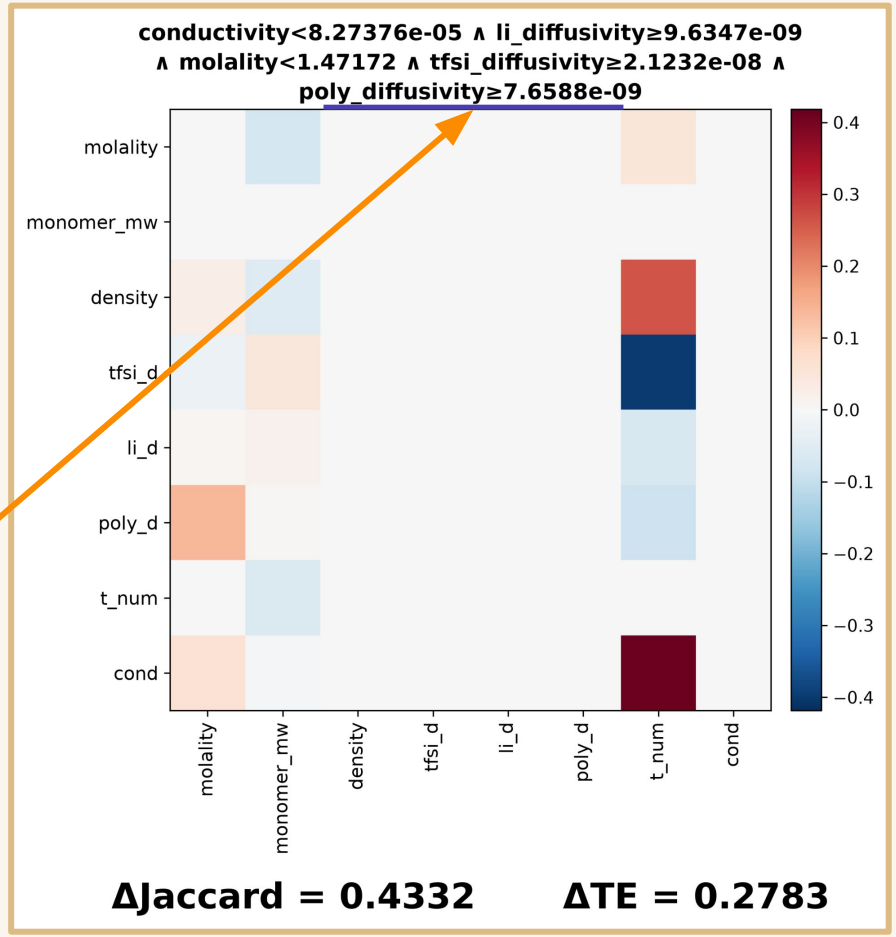
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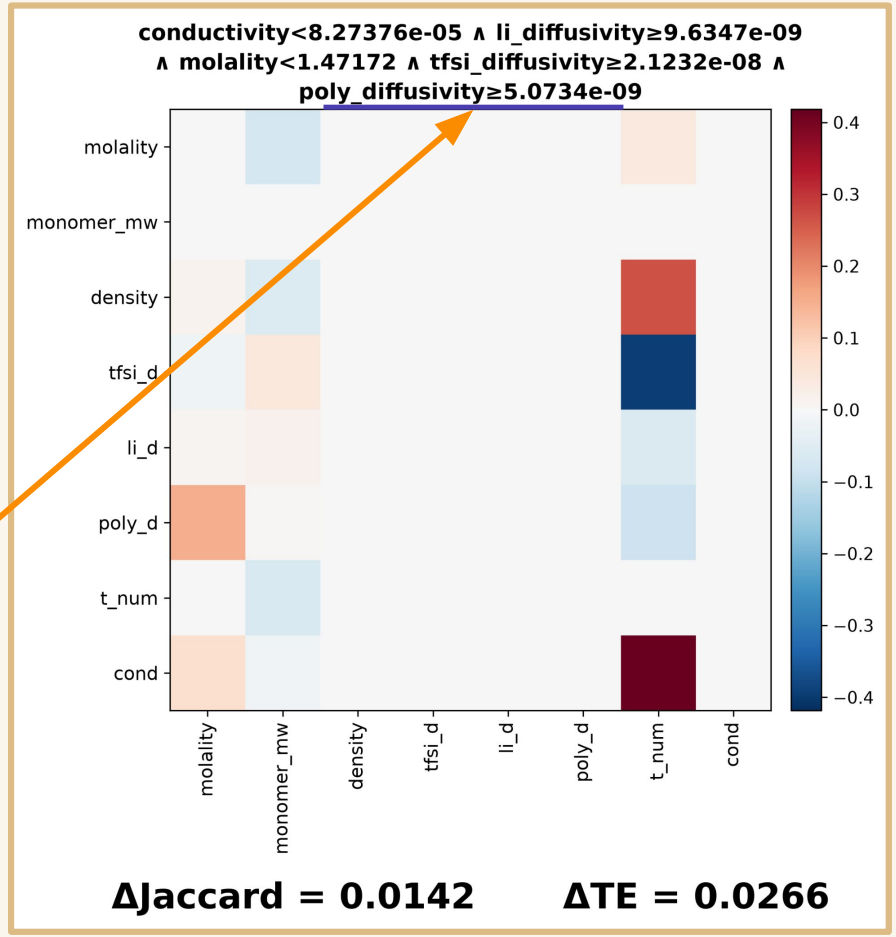
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Potential **drivers** of a fixed **mechanism**

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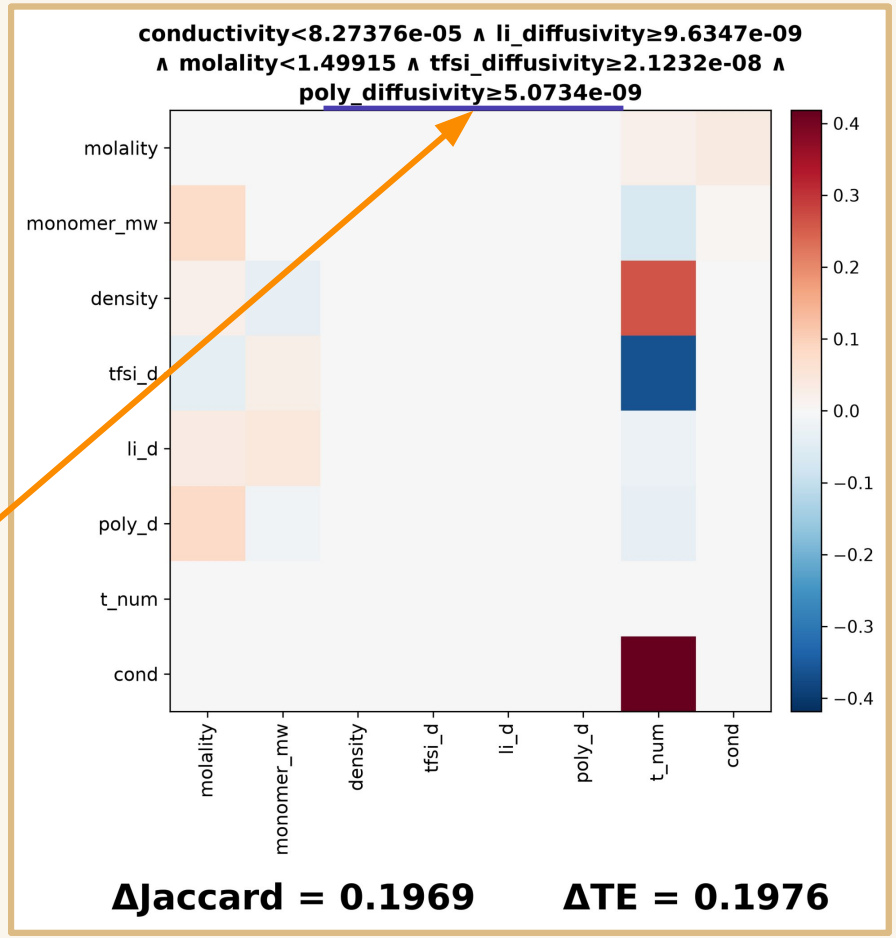
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Potential **drivers** of a fixed **mechanism**

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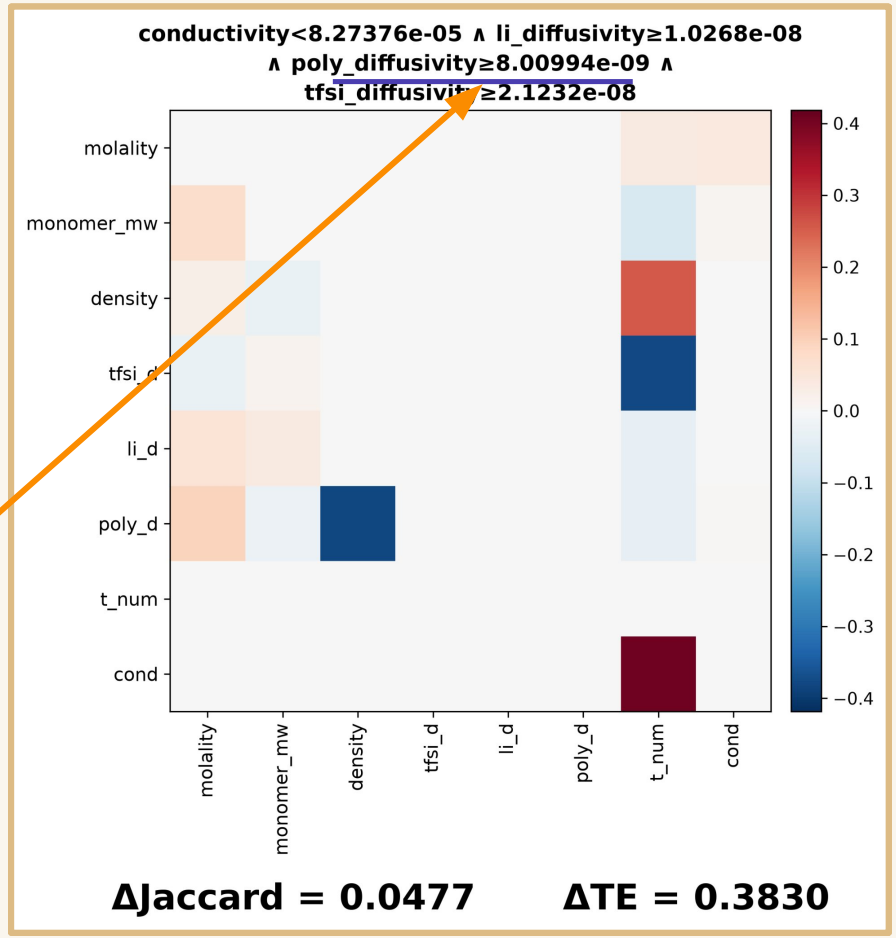
CONDITIONAL PATHING

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Some conditions are *load bearing candidates* (**conductivity, tfsi_diffusivity**)

Potential **drivers** of a fixed **mechanism**

Changes “freely”!



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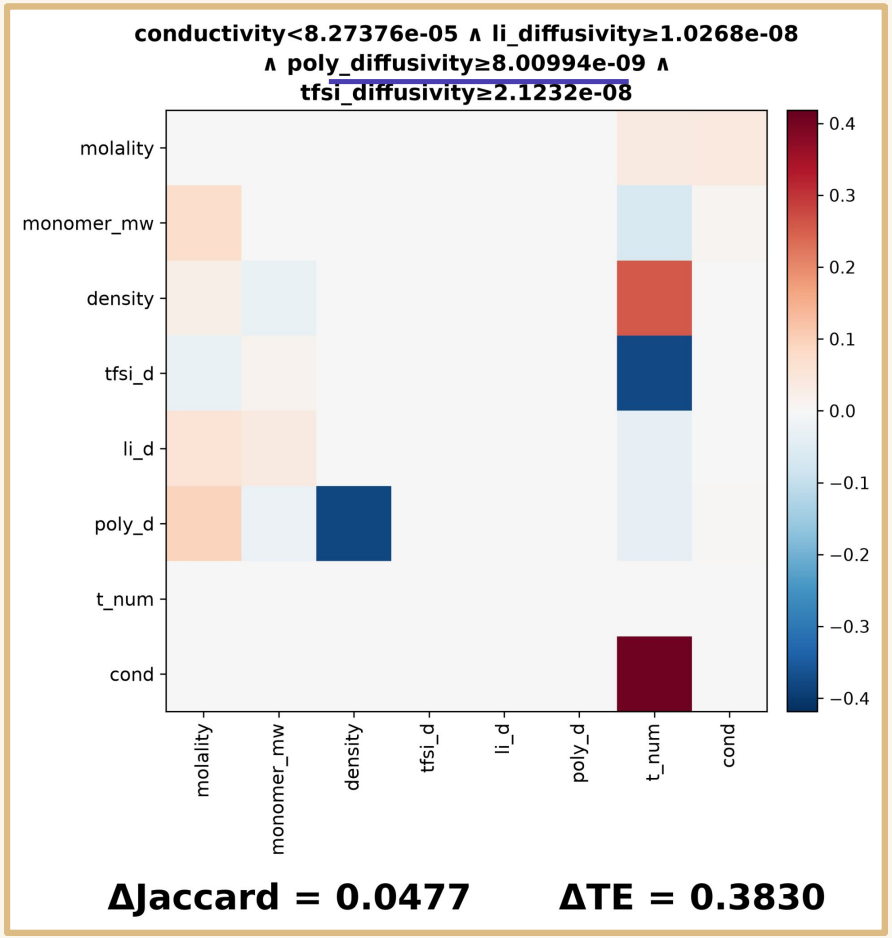
CONDITIONAL PATHING

The path algorithm

Some conditions are *load bearing candidates* (**conductivity, tfsi_diffusivity**)

Potential **drivers** of a fixed **mechanism**

Other conditions are *mechanism irrelevant candidates* (**poly_diffusivity**)



0->1->2->3->4->5->6

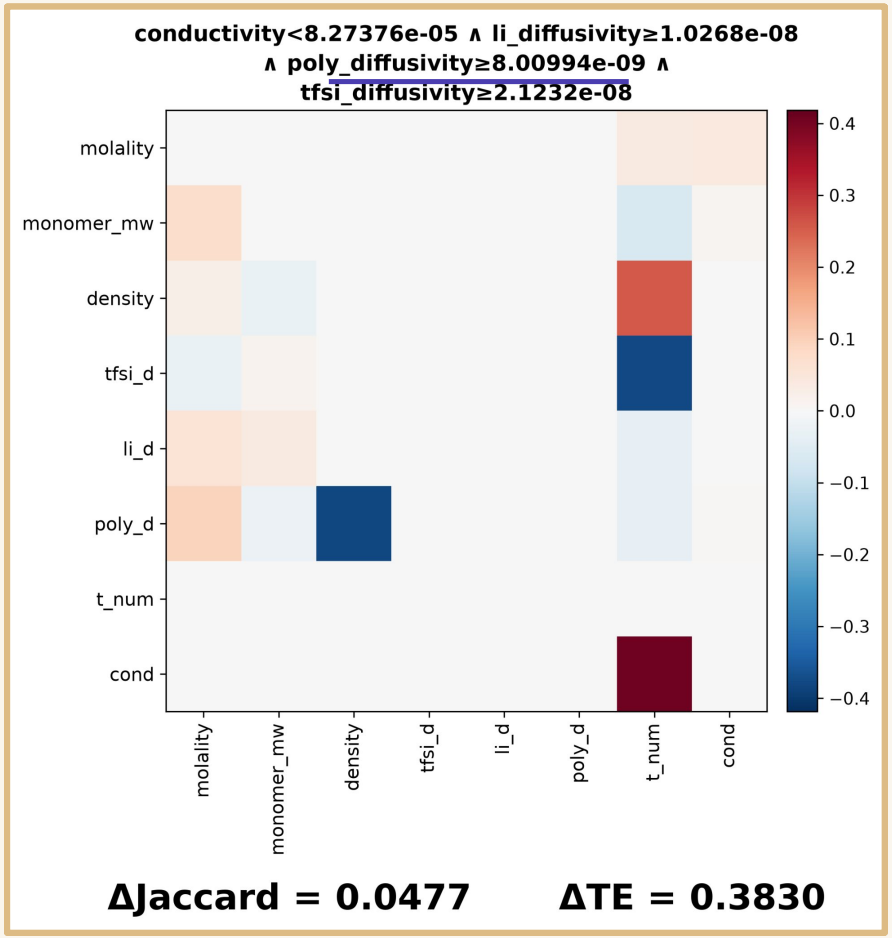
CONDITIONAL PATHING

The path algorithm

Some conditions are *load bearing candidates* (**conductivity, tfsi_diffusivity**)

Discoverability!

Other conditions are *mechanism irrelevant candidates* (**poly_diffusivity**)

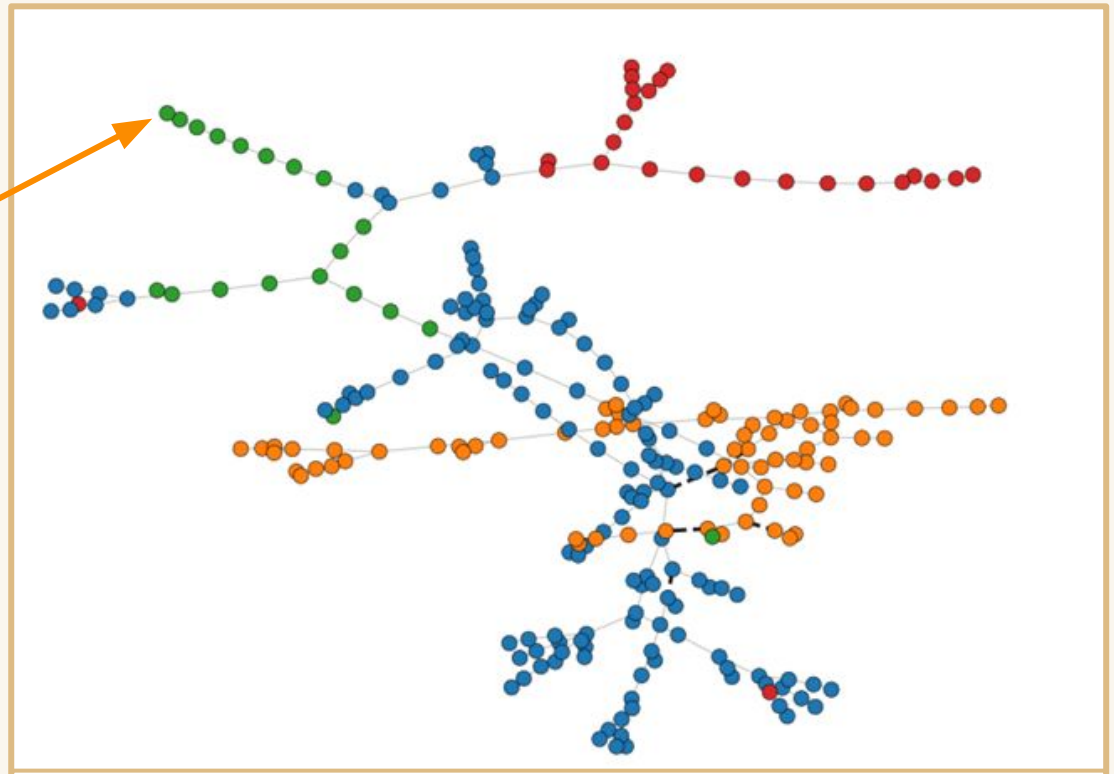


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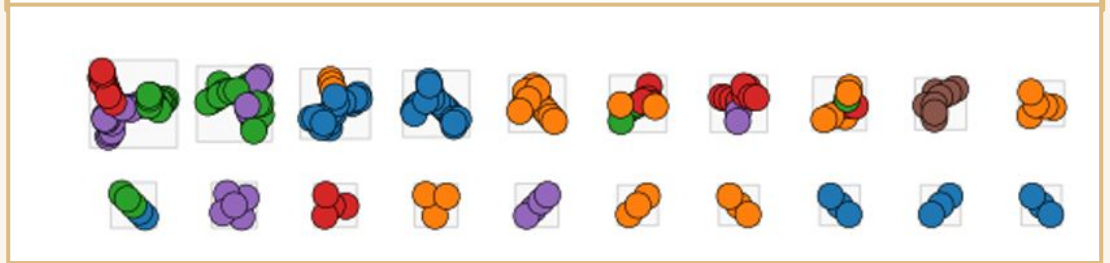
CONDITIONAL PATHING

Path Components

Each dot is a single condition-graph pair



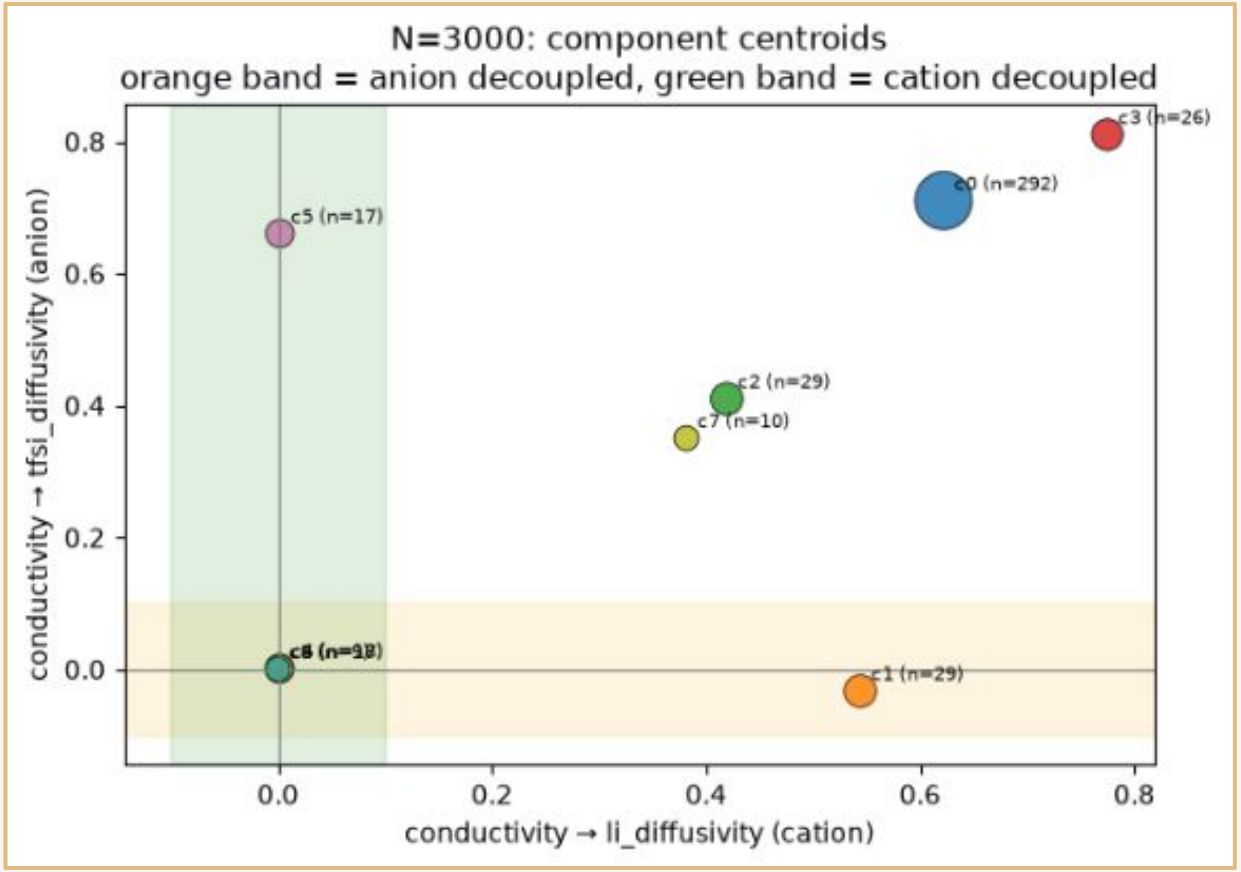
Path Components: **clustering** that respect the underlying **topologies.**



CONDITIONAL PATHING

Path Components

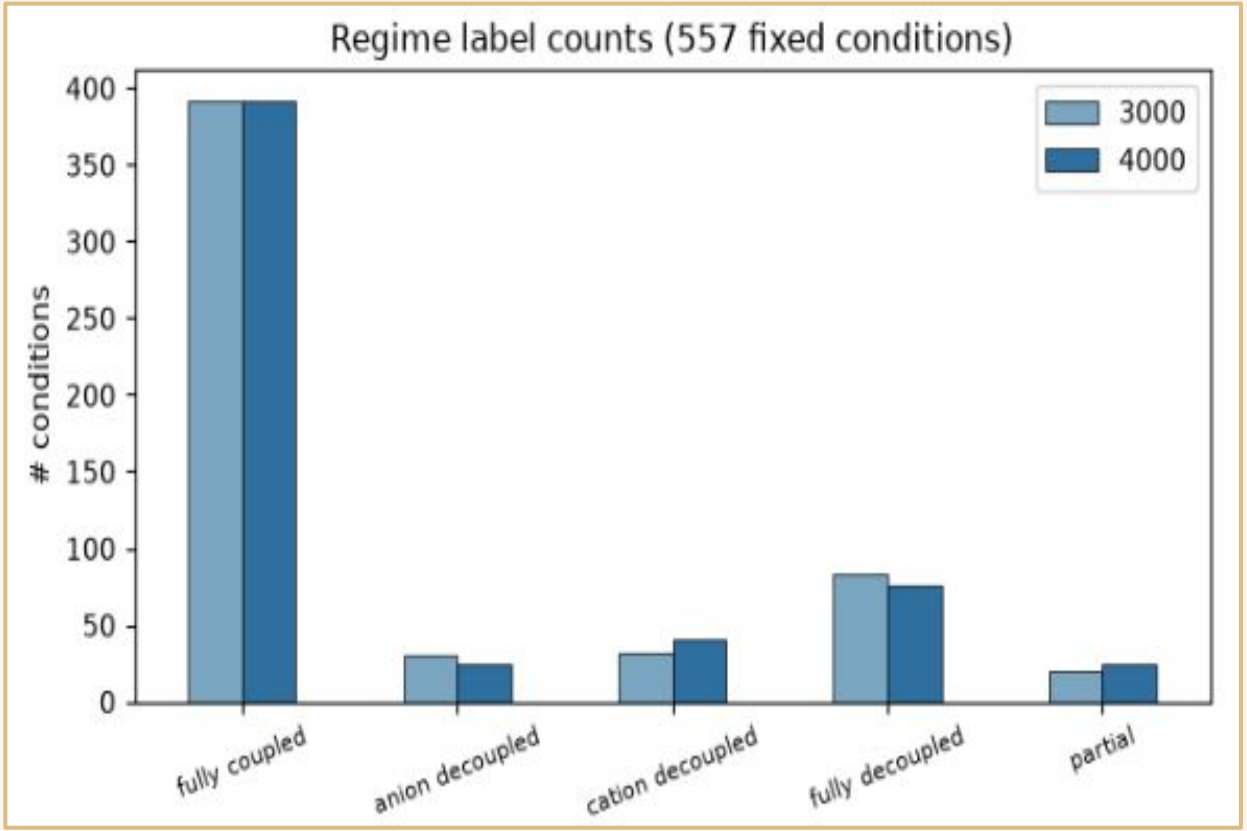
total Effect Evaluation across Clusters →
Clear Separation Identified



CONDITIONAL PATHING

Path Components

Robust Regime Distribution Across Sample Sizes *N*



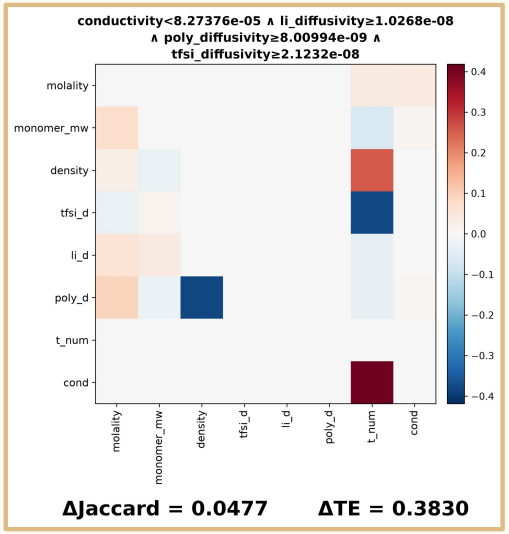
CONDITIONAL PATHING

Future Work

Explore more patterns in the paths

Study more paths

apply to **more data**.



Theoretical Guarantees

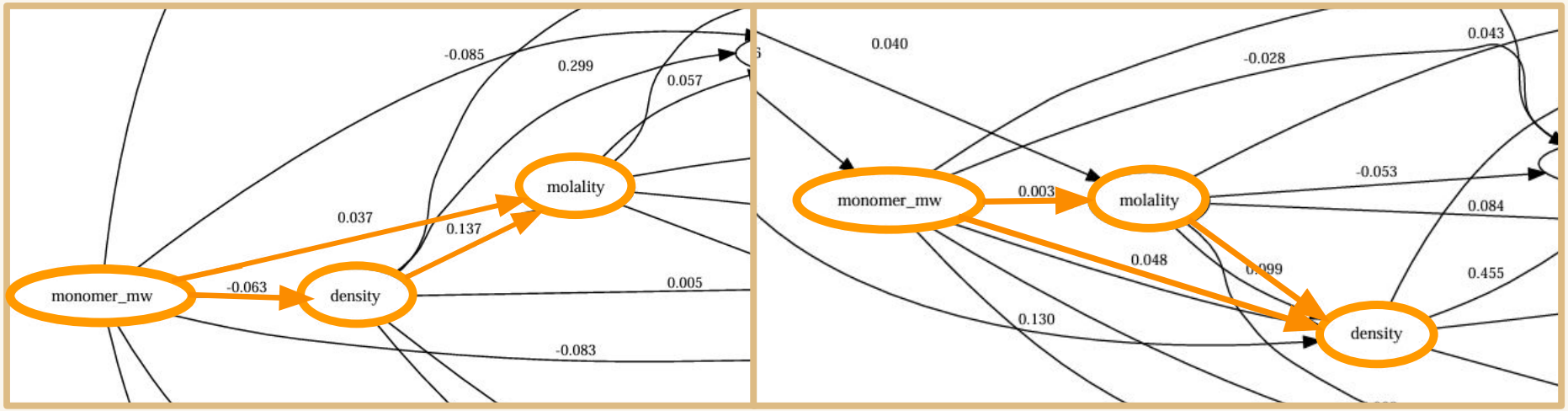
Prove our conjectures regarding the robustness of pathing.

Automate Discovery

Automate detection of *mechanism irrelevancies* and *load bearing candidates* in relevant paths.

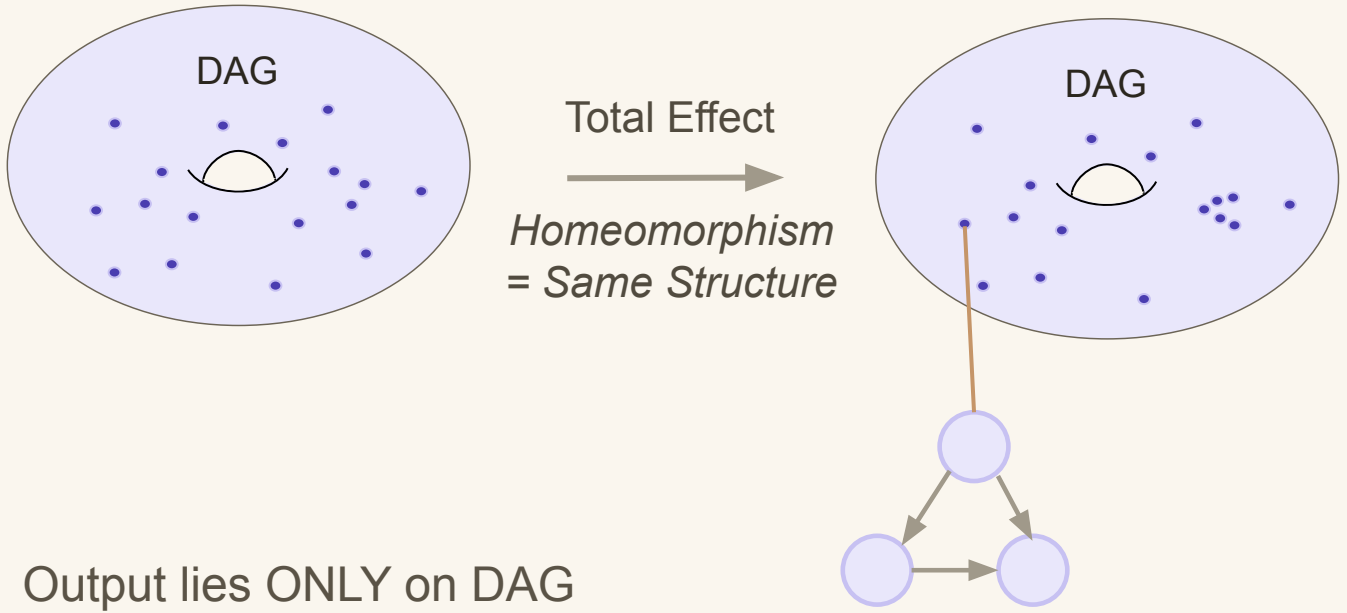
LOCA PATHING

Local Pathing



Study **substructures** as conditions change

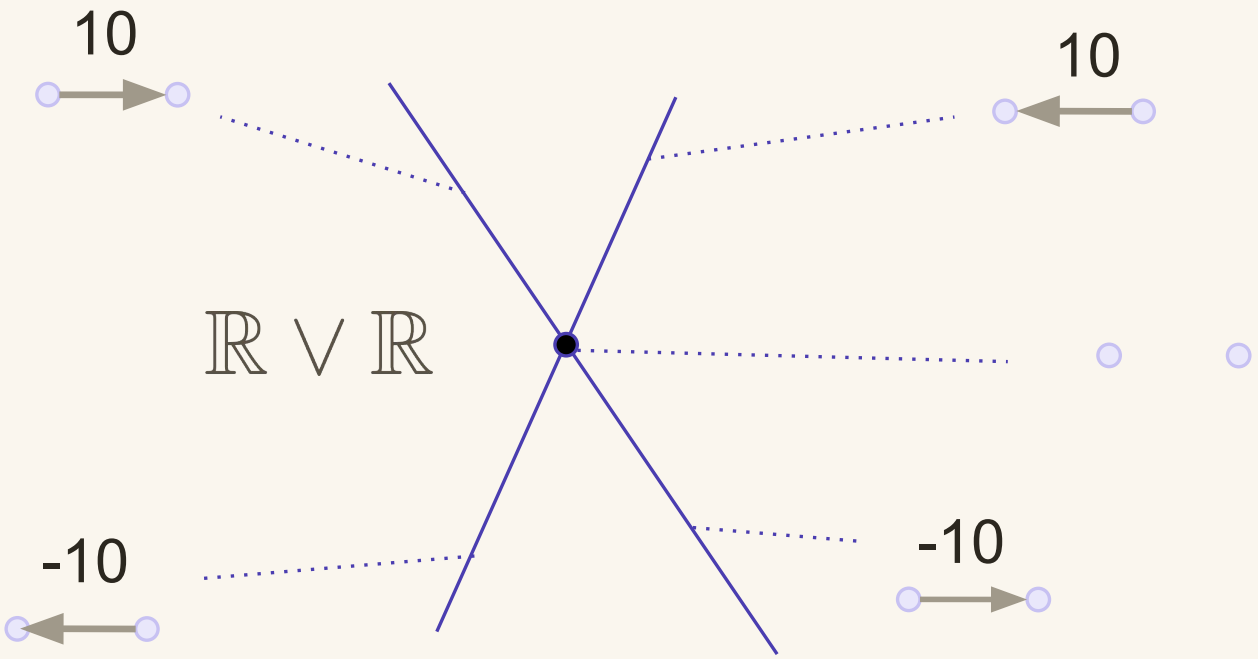
Underlying Topology



Output lies ONLY on DAG

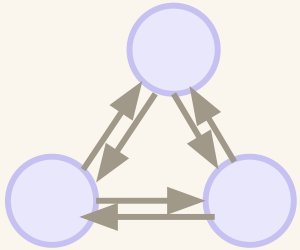
LOCAL PATHING

Edge Space



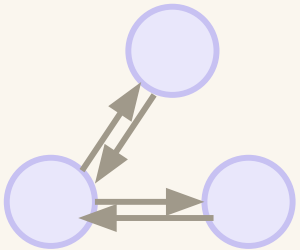
All possibilities between fixed nodes

Nerve Structure of Topology



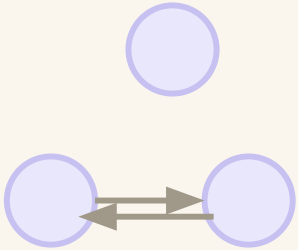
“point”

$(\mathbb{R} \vee \mathbb{R})^3$



“edge”

$(\mathbb{R} \vee \mathbb{R})^2$



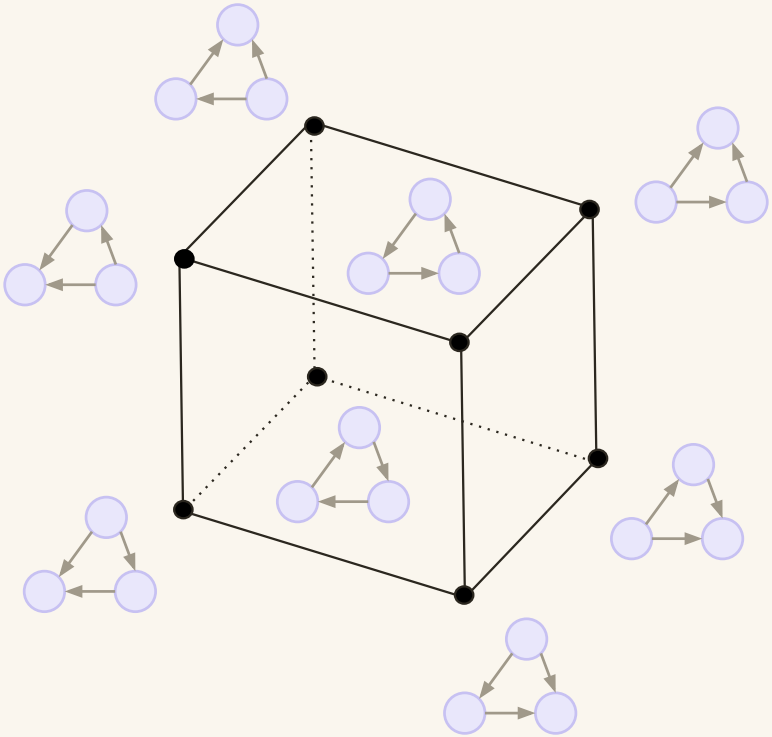
“face”

$\mathbb{R} \vee \mathbb{R}$

All edge + weight possibilities

LOCAL PATHING

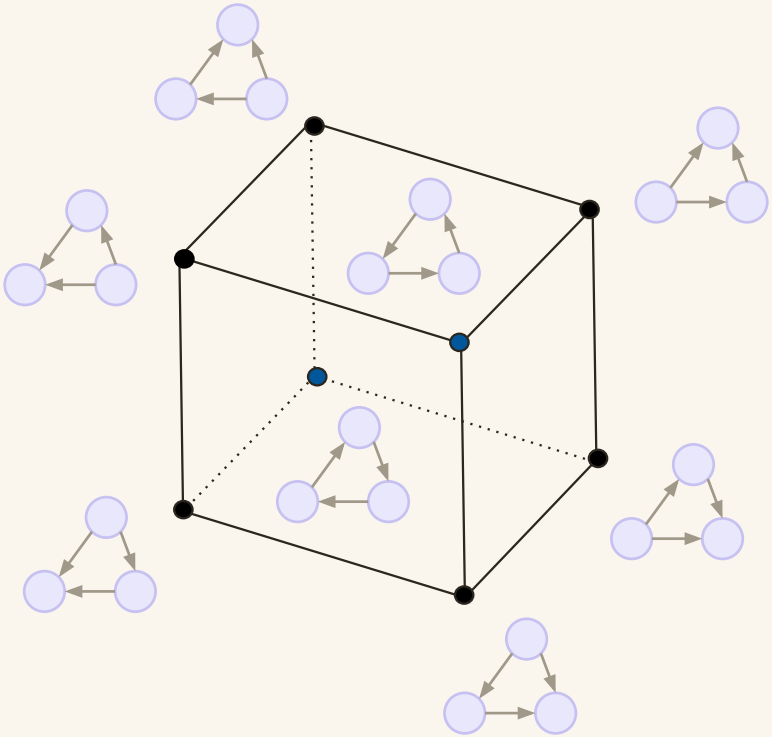
3-node Pathing



Small example

LOCAL PATHING

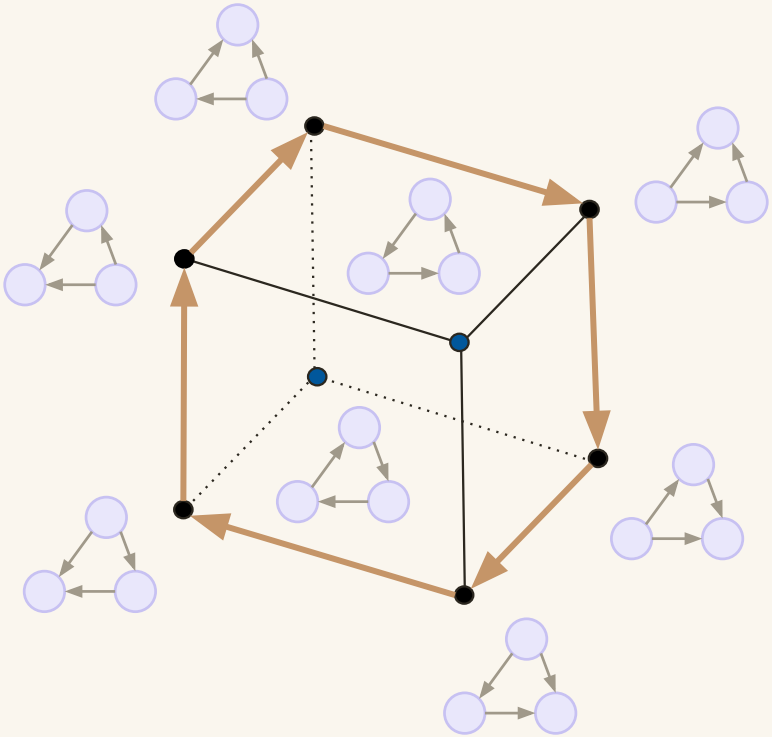
3-node Pathing



- Remove cycles

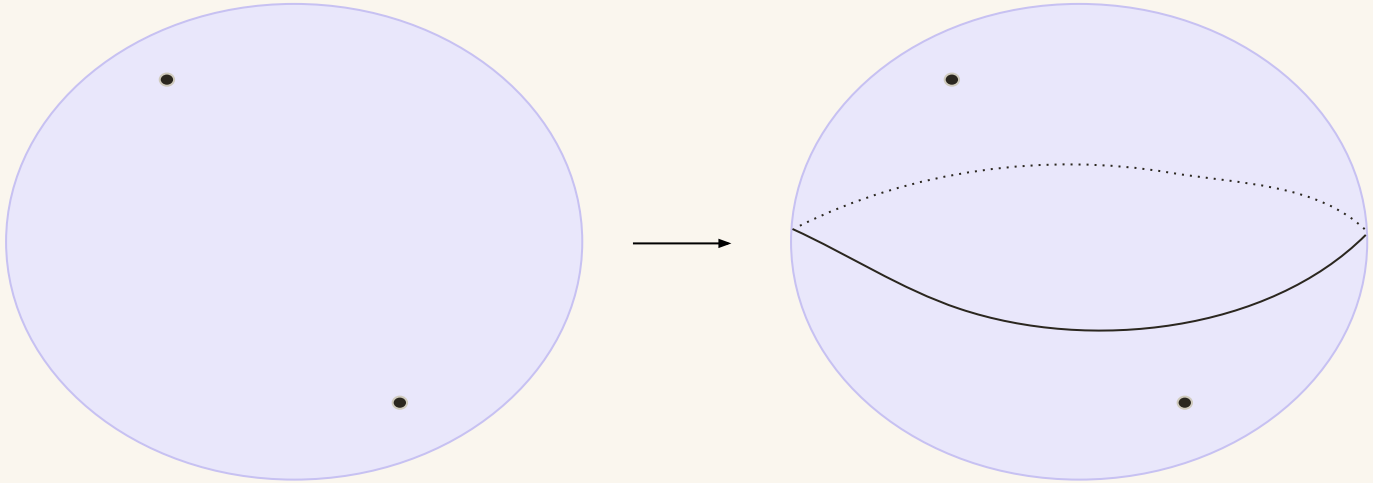
LOCAL PATHING

3-node Pathing



Consider loop in DAG space

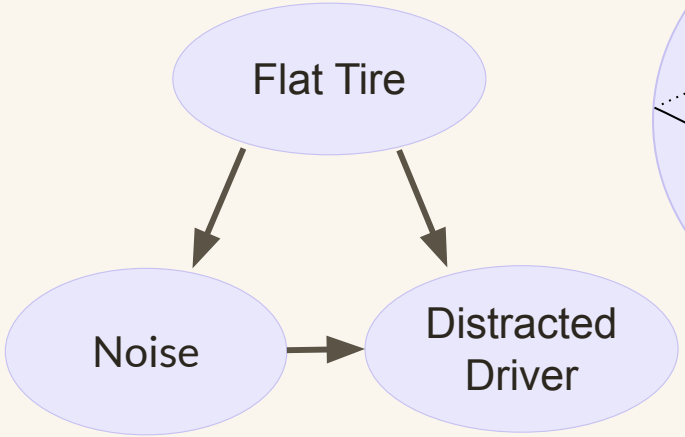
Choice of Object to Study

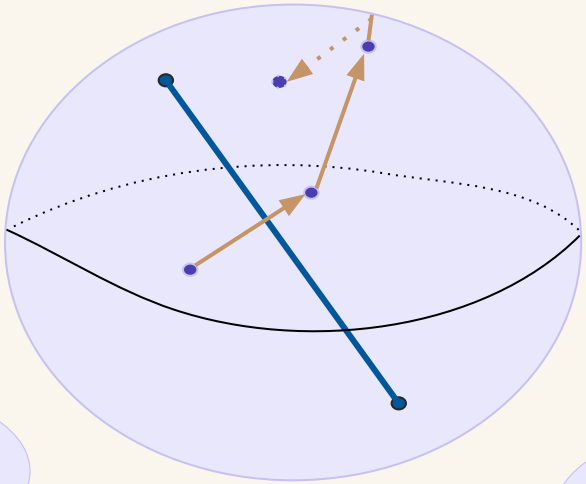


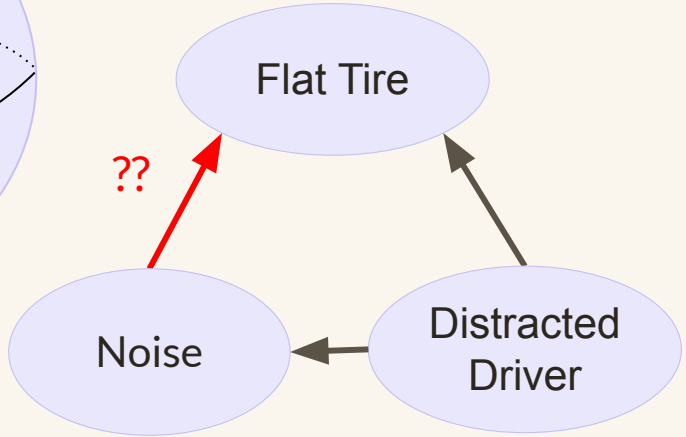
$$L_n = S^{n(n-1)-1} \cap \mathrm{DAG}_n$$

Remove 0!

3-node Toy Example







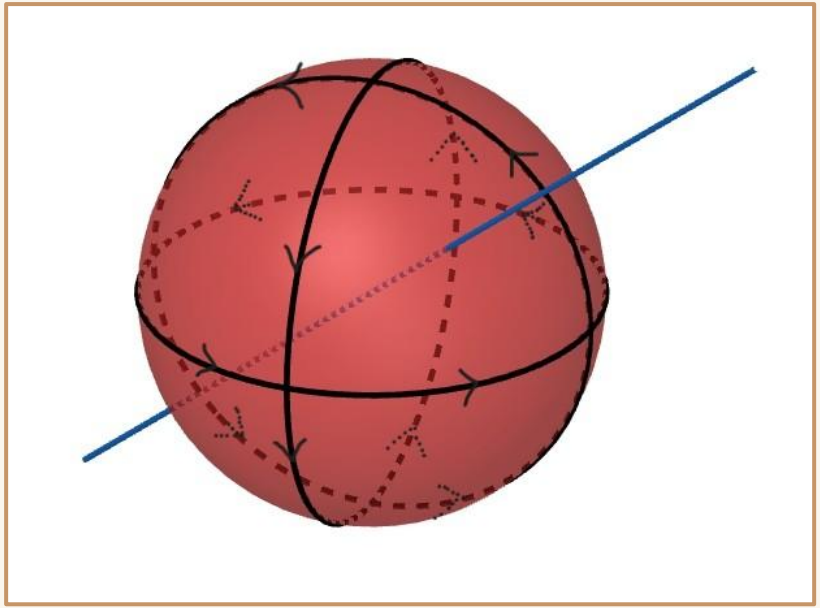
Causal graphs “wind” around this line
Half loops may represent incongruence

Projecting Along Cycles

$$M \mapsto M|_{P_{CW}}, M|_{P_{CCW}}$$

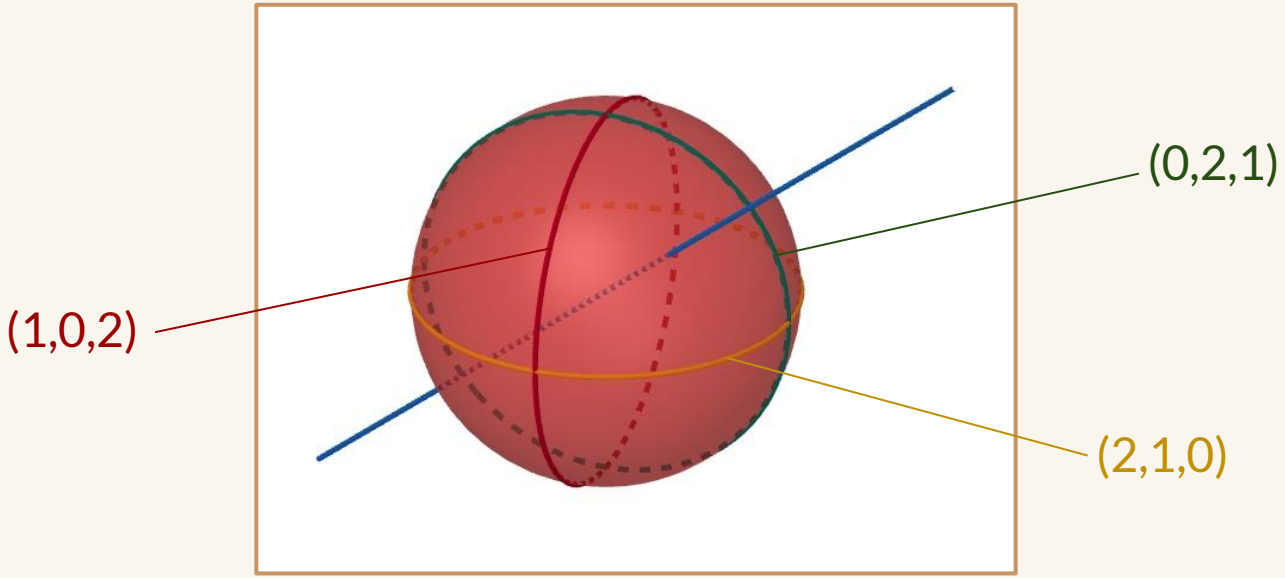
$$P_{CW} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, P_{CCW} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$M|_{P_{CW}}, M|_{P_{CCW}} \mapsto \mathrm{Norm}(M|_{P_{CW}}), \mathrm{Norm}(M|_{P_{CCW}})$$



Consider several projections on choice of 3 columns

Projecting Along Cycles (Causal Order)



Graphs with cyclic sub-causal order lie on 3 great circles

3-Node Pathing Algorithm

$$\{p_0, p_1, \ldots\} \quad \max_{p_{i+1} \in C_{p_i}} (\theta(p_i, p_{i+1})) - d_J(p_i, p_{i+1})) : d_J < \epsilon = c \cdot \text{mean}(d_J)$$

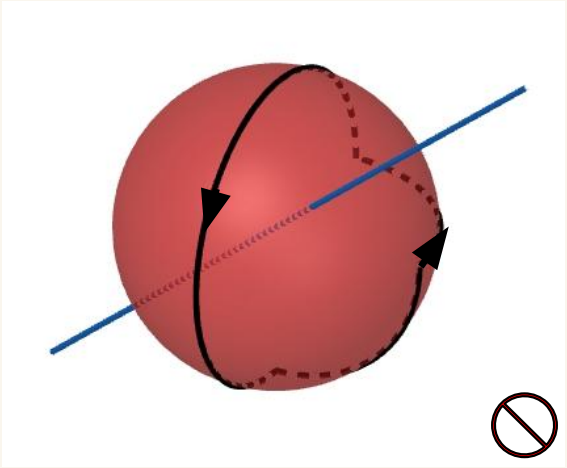
Incremental Winding

Incremental Jaccard

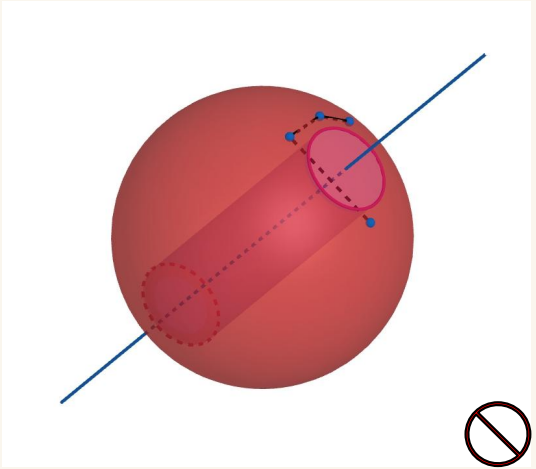
> Winding algorithm conditions

3-Node Pathing Algorithm

1) No returning to great circles



2) Avoid cylinder about line

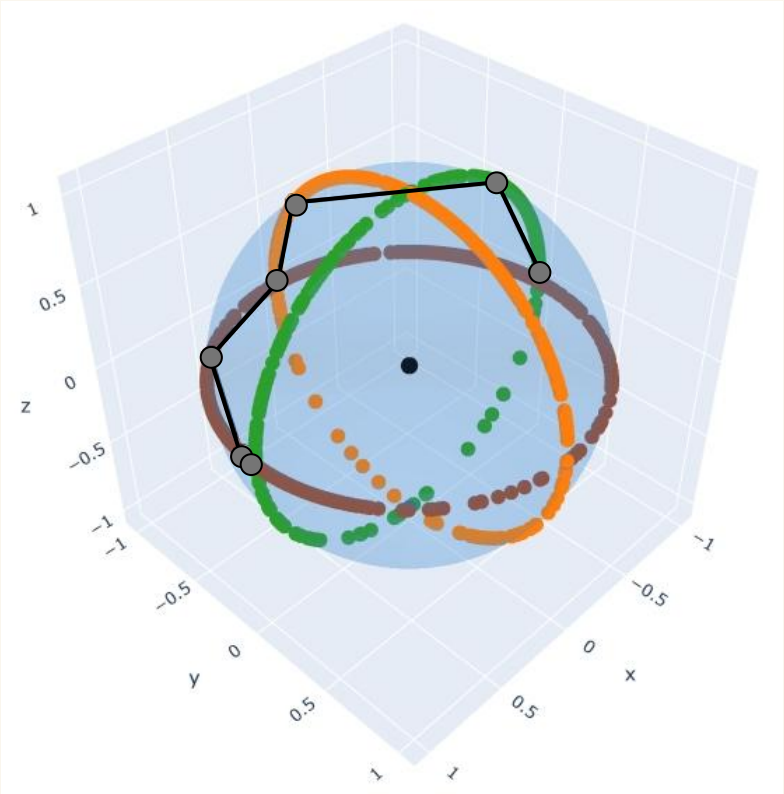


Winding algorithm conditions

LOCAL PATHING

3-Node Pathing on Real Data

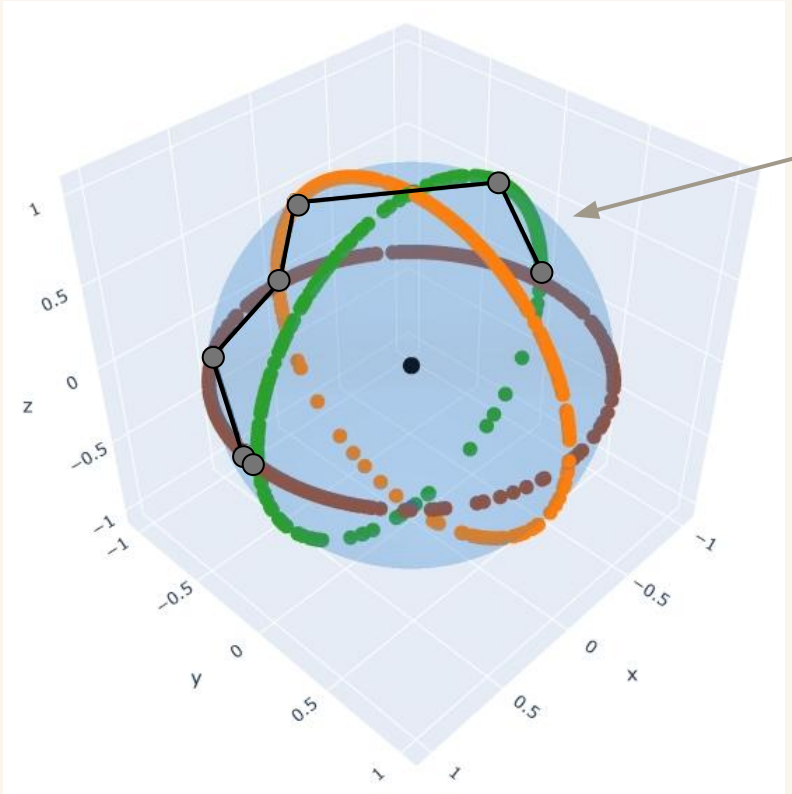
Winding on real data; Jaccard threshold 0.3 of mean



LOCAL PATHING

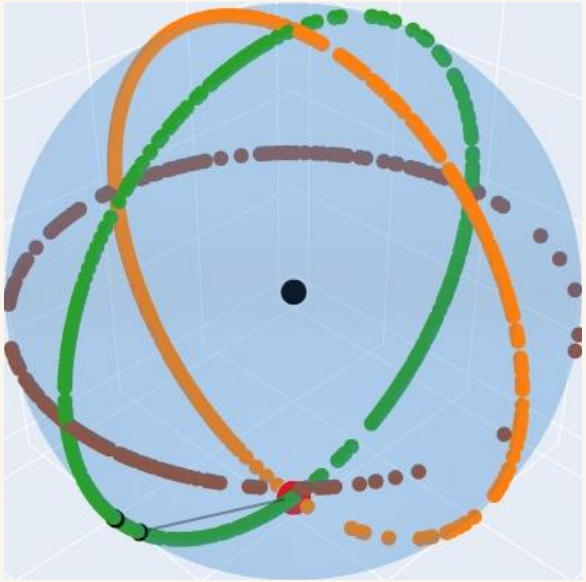
3-Node Pathing on Real Data

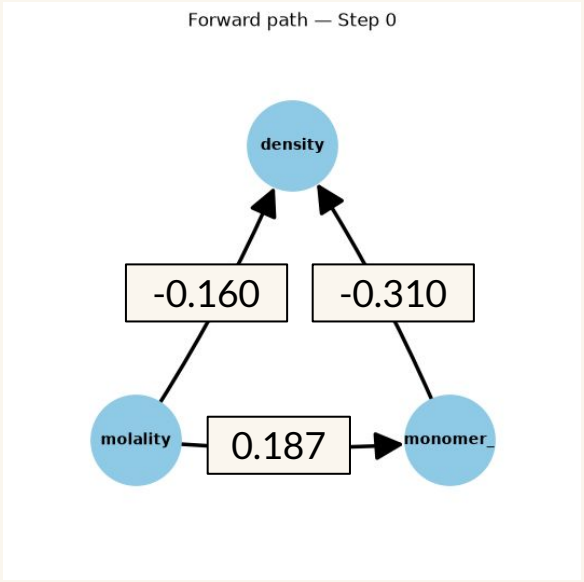
Winding on real data; Jaccard threshold 0.3 of mean



LOCAL PATHING

3-Node Pathing (Small Jaccard)

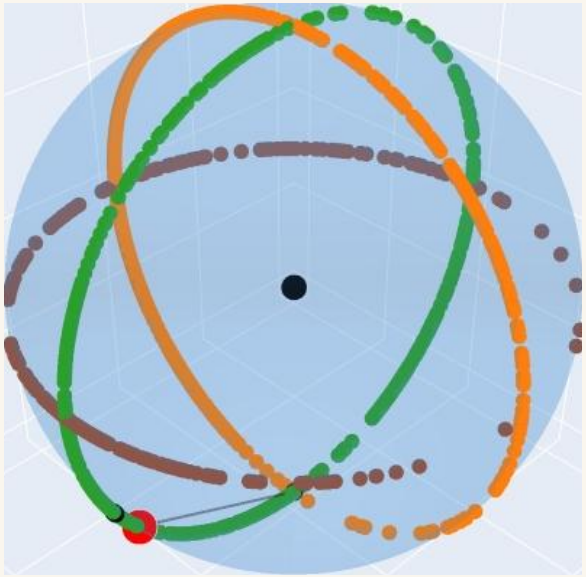


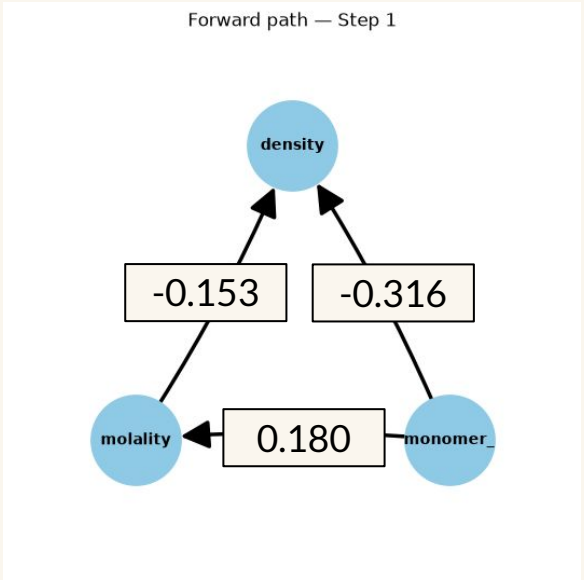


Forward - Step 0; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing (Small Jaccard)

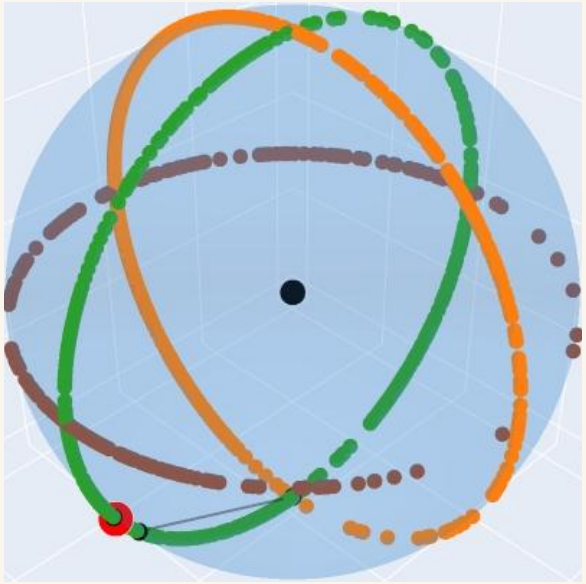


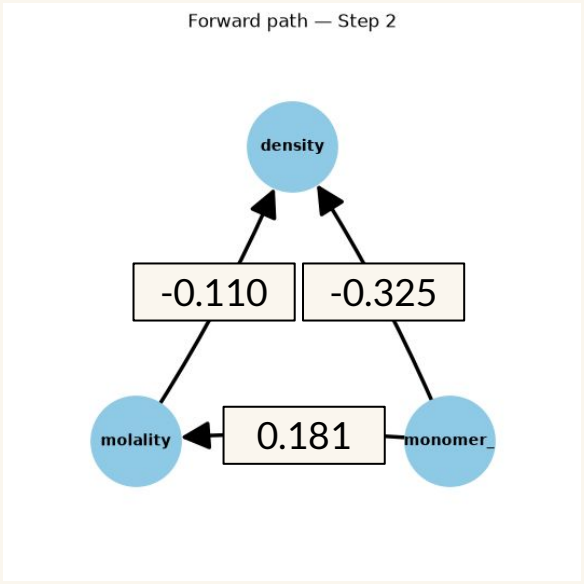


Forward - Step 1; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing (Small Jaccard)

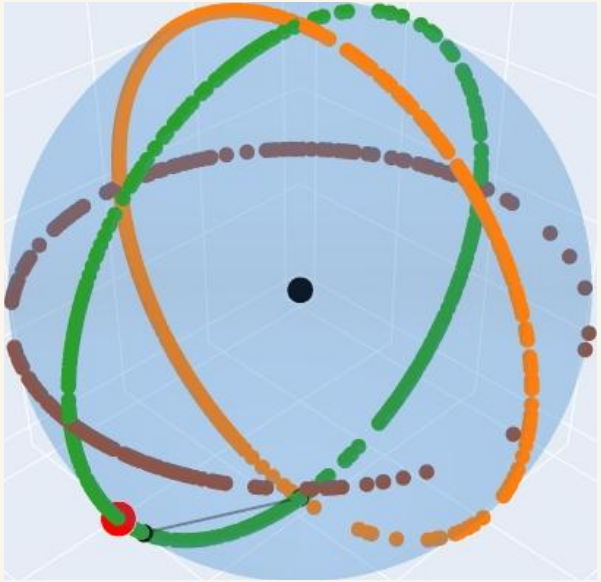


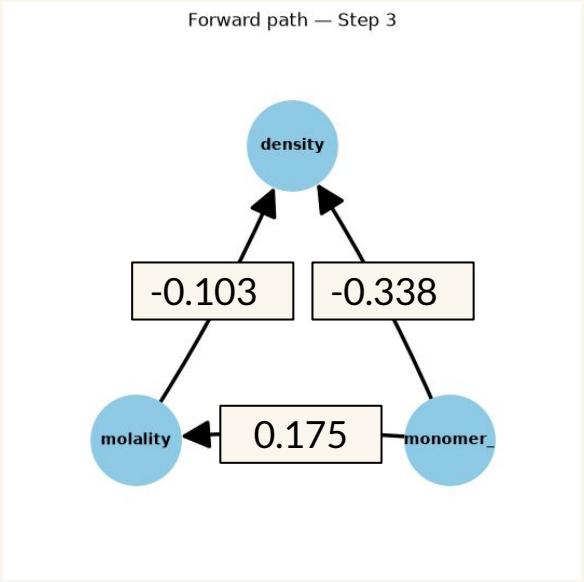


Forward - Step 2; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing (Small Jaccard)

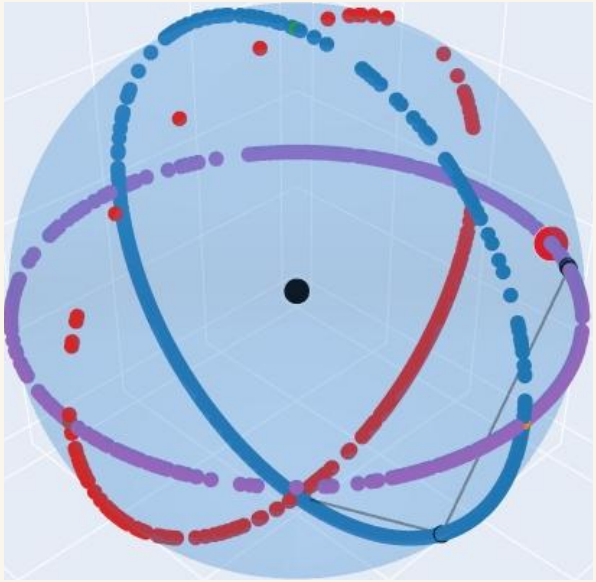


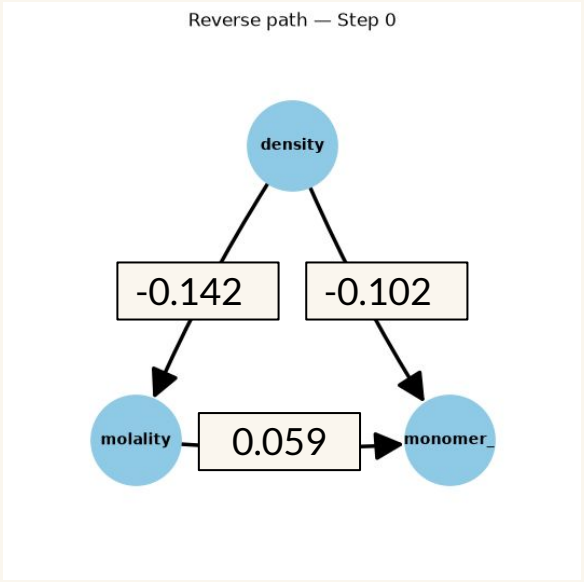


Forward - Step 3; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing (Small Jaccard)

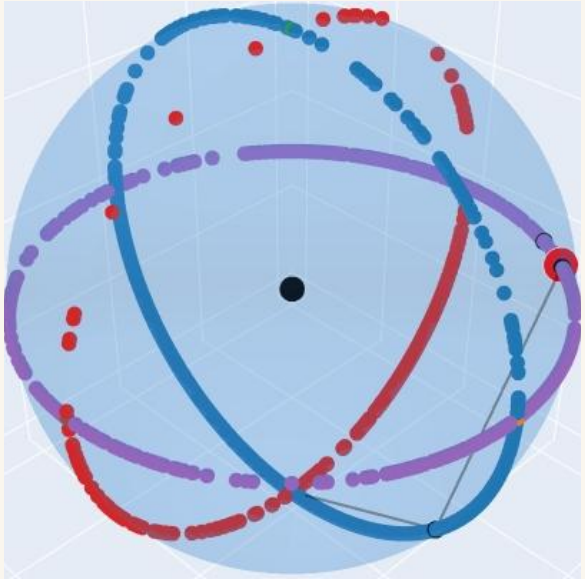


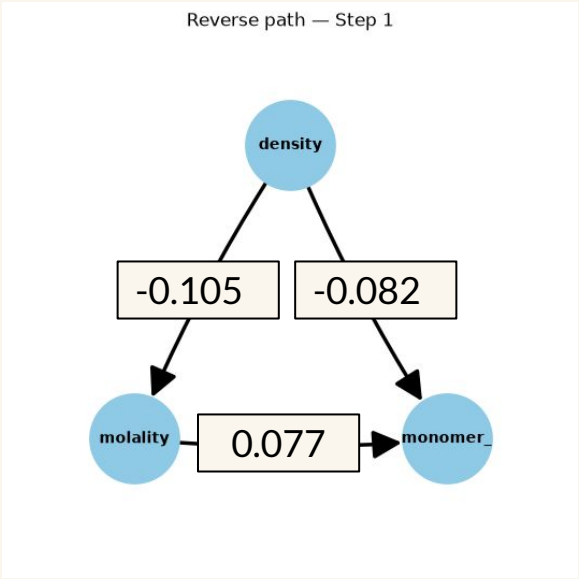


Backward- Step 0; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing (Small Jaccard)

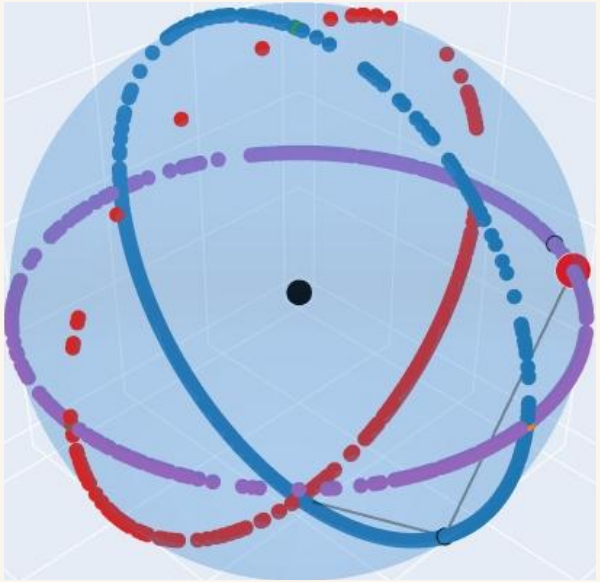


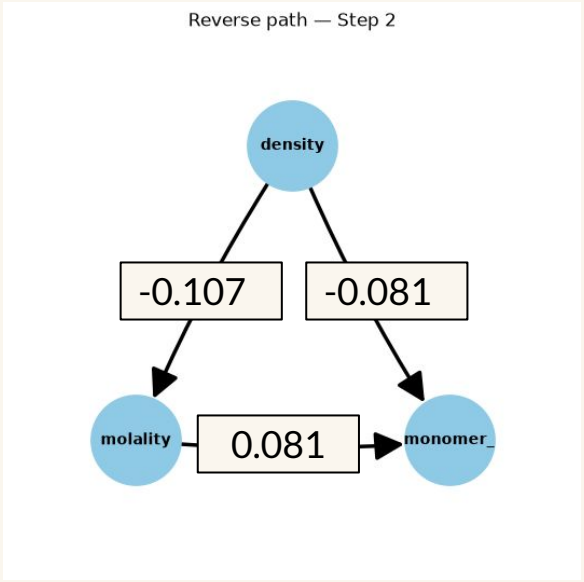


Backward- Step 1; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing (Small Jaccard)

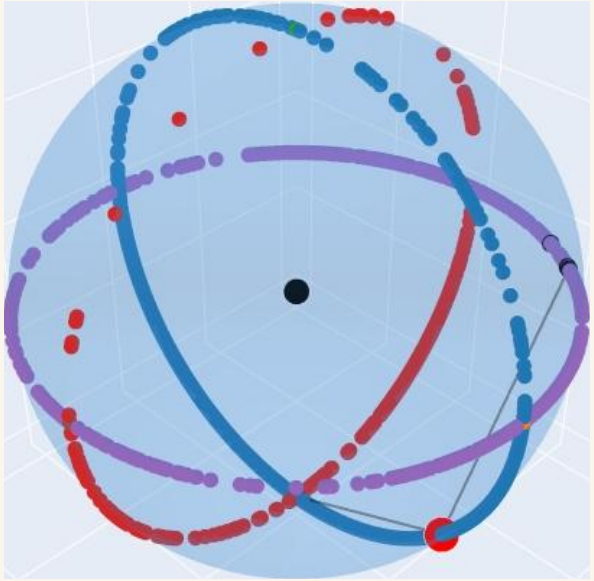


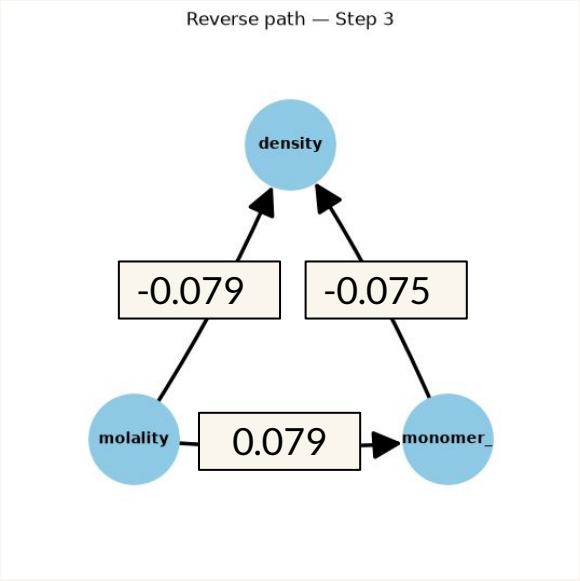


Backward- Step 2; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing (Small Jaccard)

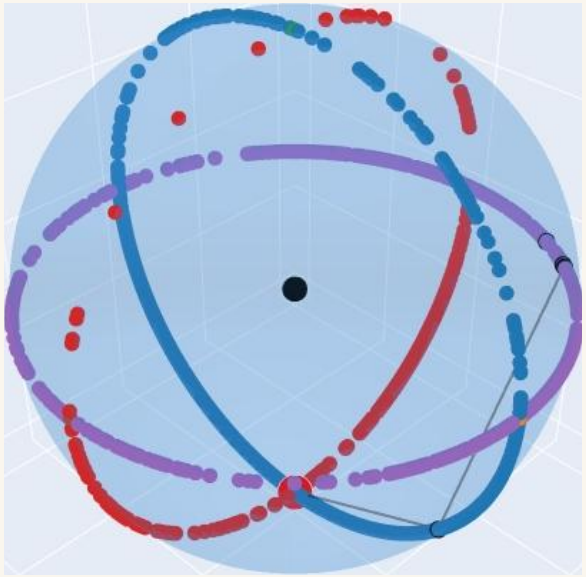


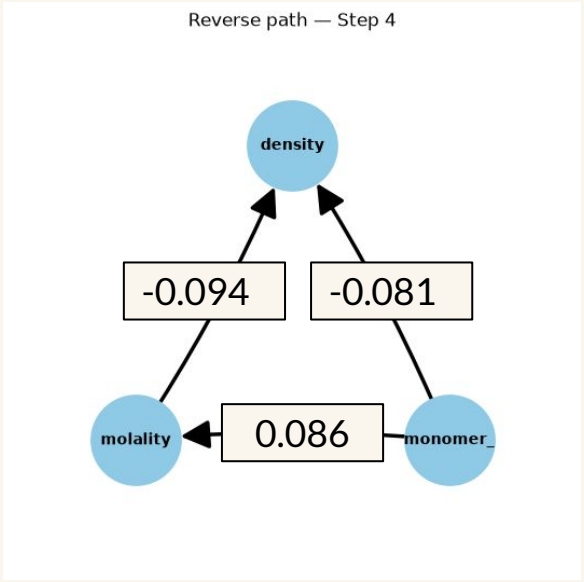


Backward- Step 3; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing (Small Jaccard)





Backward- Step 4; Jaccard threshold 0.1 of mean

LOCAL PATHING

3-Node Pathing Full Data

Forward			Reverse		
Columns	Winding	Len	Columns	Winding	Len
(M, Li, TN)	1.653	3	(M, MW, D)	1.756	5
(M, MW, TN)	1.573	5	(M, Li, TN)	1.570	5
(MW, D, Li)	1.545	3	(M, MW, TN)	1.217	3
(D, Li, TN)	1.309	3	(M, D, TN)	1.18	3
(D, TN, Cond)	1.074	2	(Li, Poly, TN)	1.18	3
(M, D, TN)	1.051	2	(D, Li, TN)	1.149	3
(MW, TN, Cond)	1.013	4	(M, MW, Cond)	1.132	2
(M, MW, Cond)	0.989	3	(MW, D, Cond)	1.066	2
(TFSI, Poly, TN)	0.892	3	(M, TFSI, Cond)	1.047	4
(MW, Poly, TN)	0.882	4	(TFSI, Li, TN)	1.047	3
(MW, TFSI, Poly)	0.864	4	(MW, Poly, TN)	1.047	4
(M, D, Cond)	0.810	3	(MW, TFSI, Cond)	1.010	3
(MW, D, TN)	0.794	2	(M, Poly, TN)	0.955	2
(M, D, Poly)	0.761	3	(M, TFSI, TN)	0.937	3
(MW, TFSI, Li)	0.732				
(Li, Poly, TN)	0.729				
(D, TFSI, Li)	0.706				
(M, MW, Poly)	0.700	3	(M, MW, Poly)	0.809	2
(M, MW, D)	0.673	4	(M, MW, Li)	0.770	3
(MW, Li, TN)	0.671	7	(MW, TFSI, TN)	0.754	4
(M, Li, Poly)	0.613	3	(D, TFSI, Cond)	0.734	4
(TFSI, TN, Cond)	0.609	3	(D, Poly, TN)	0.714	4
(TFSI, Li, TN)	0.605	2	(MW, Li, TN)	0.702	3
(M, TN, Cond)	0.600	2	(M, D, Poly)	0.698	3
(D, Li, Poly)	0.592	4	(D, TFSI, TN)	0.661	3
(M, Poly, Cond)	0.579	2	(MW, Li, Poly)	0.648	3
(D, TFSI, Cond)	0.577	2	(TFSI, Li, Poly)	0.643	2
(Poly, TN, Cond)	0.565	2	(M, Li, Cond)	0.640	4

(M, MW, D) 1.756 5

(M, MW, D) 0.673 4

(D, TFSI, Poly)	0.554	2	(D, Poly, Cond)	0.638	4
(MW, D, Cond)	0.543	2	(M, D, Li)	0.622	2
(TFSI, Li, Poly)	0.534	2	(TFSI, TN, Cond)	0.612	3
(M, D, Li)	0.533	2	(MW, TN, Cond)	0.599	2
(M, Poly, TN)	0.531	2	(D, TFSI, Li)	0.588	3
					2
					2
					4
(TFSI, Poly, Cond)	0.489	2	(MW, D, Li)	0.526	2
(M, Li, Cond)	0.478	2	(M, Li, Poly)	0.519	2
(D, Poly, TN)	0.460	2	(D, TN, Cond)	0.515	2
(M, TFSI, Cond)	0.457	2	(M, Poly, Cond)	0.510	2
(Li, Poly, Cond)	0.422	2	(D, Li, Cond)	0.498	2
(M, TFSI, Poly)	0.410	2	(TFSI, Poly, TN)	0.488	2
(D, Li, Cond)	0.380	2	(TFSI, Li, Cond)	0.471	2
(D, TFSI, TN)	0.374	5	(D, TFSI, Poly)	0.452	2
			oly)	0.446	2
			Cond)	0.424	2
(Li, TN, Cond)	0.312	2	(M, TFSI, Li)	0.348	2
(TFSI, Li, Cond)	0.311	2	(MW, Li, Cond)	0.330	2
(D, Poly, Cond)	0.307	2	(MW, TFSI, Poly)	0.277	2
(MW, Poly, Cond)	0.295	2	(TFSI, Poly, Cond)	0.273	3
(M, TFSI, TN)	0.265	3	(M, D, TFSI)	0.245	2
(M, D, TFSI)	0.252	2	(MW, D, Poly)	0.213	2
(MW, TFSI, TN)	0.250	2	(MW, D, TFSI)	0.163	2
(M, TFSI, Li)	0.211	2	(Li, TN, Cond)	0.124	2
(MW, TFSI, Cond)	0.196	2	(MW, TFSI, Li)	0.111	2
(MW, Li, Cond)	0.169	2	(Li, Poly, Cond)	0.095	2

Ranked winding (Molality, Monomer Width, Density)

3-Node Pathing Full Data

Forward			Reverse		
Columns	Winding	Len	Columns	Winding	Len
(M, Li, TN)	1.653	3	(M, MW, D)	1.756	5
(M, MW, TN)	1.573	5	(M, Li, TN)	1.570	5
(MW, D, Li)	1.545	3	(M, MW, TN)	1.217	3
(D, Li, TN)	1.309	3	(M, D, TN)	1.189	3
(D, TN, Cond)	1.074	2	(Li, Poly, TN)	1.182	2
(M, D, TN)	1.051	2	(D, Li, TN)	1.149	3
(MW, TN, Cond)	1.013	4	(M, MW, Cond)	1.132	2
(M, M					
(TFSI					
(MW, Poly, TN)	0.882	4	(TFSI, Li, TN)	1.047	3
(MW, TFSI, Poly)	0.864	4	(MW, Poly, TN)	1.047	4
(M, D, Cond)	0.810	3	(MW, TFSI, Cond)	1.010	3
(Li, Poly, TN)	0.729	3	(M, TN, Cond)	0.873	3
(D, TFSI, Li)	0.706	3	(MW, D, TN)	0.828	3
(M, MW, Poly)	0.700	3	(M, MW, Poly)	0.809	2
(M, MW, D)	0.673	4	(M, MW, Li)	0.770	3
(MW, Li, TN)	0.671	7	(MW, TFSI, TN)	0.754	4
(M, Li, Poly)	0.613	3	(D, TFSI, Cond)	0.734	4
(TFSI, TN, Cond)	0.609	3	(D, Poly, TN)	0.714	4
(TFSI, Li, TN)	0.605	2	(MW, Li, TN)	0.702	3
(M, TN, Cond)	0.600	2	(M, D, Poly)	0.698	3
(D, Li, Poly)	0.592	4	(D, TFSI, TN)	0.661	3
(M, Poly, Cond)	0.579	2	(MW, Li, Poly)	0.648	3
(D, TFSI, Cond)	0.577	2	(TFSI, Li, Poly)	0.643	2
(Poly, TN, Cond)	0.565	2	(M, Li, Cond)	0.640	4

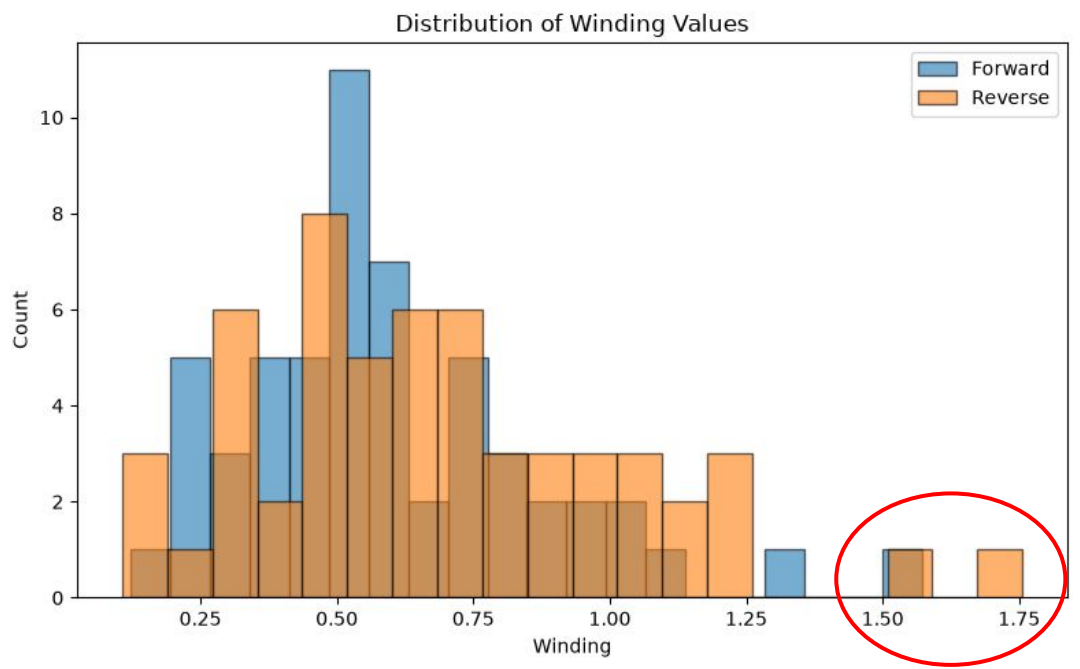
(TFSI, Li, Cond) 0.471 2

(TFSI, Li, Cond) 0.311 2

(D, TFSI, Poly)	0.554	2	(D, Poly, Cond)	0.638	4
(MW, D, Cond)	0.543	2	(M, D, Li)	0.622	2
(TFSI, Li, Poly)	0.534	2	(TFSI, TN, Cond)	0.612	3
(M, D, Li)	0.533	2	(MW, TN, Cond)	0.599	2
(M, Poly, TN)	0.531	2	(D, TFSI, Li)	0.588	3
(MW, D, TFSI)	0.521	3	(D, Li, Poly)	0.577	2
(MW, D, Poly)	0.516	2	(M, MW, TFSI)	0.550	2
(M, MW, Li)	0.505	2	(Poly, TN, Cond)	0.543	4
(TFSI, Poly, Cond)	0.489	2	(MW, D, Li)	0.526	2
		2	(M, Li, Poly)	0.519	2
		2	(D, TN, Cond)	0.515	2
(M, TFSI, Cond)	0.457	2	(M, Poly, Cond)	0.510	2
(Li, Poly, Cond)	0.422	2	(D, Li, Cond)	0.498	2
(M, TFSI, Poly)	0.410	2	(TFSI, Poly, TN)	0.488	2
ond)	0.380	2	(TFSI, Li, Cond)	0.471	2
, TN)	0.374	5	(D, TFSI, Poly)	0.452	2
TFSI)	0.324	2	(M, TFSI, Poly)	0.446	2
(MW, Li, Poly)	0.321	3	(MW, Poly, Cond)	0.424	2
(Li, TN, Cond)	0.312	2	(M, TFSI, Li)	0.348	2
(TFSI, Li, Cond)	0.311	2	(MW, Li, Cond)	0.330	2
(D, Poly, Cond)	0.307	2	(MW, TFSI, Poly)	0.277	2
(MW, Poly, Cond)	0.295	2	(TFSI, Poly, Cond)	0.273	3
(M, TFSI, TN)	0.265	3	(M, D, TFSI)	0.245	2
(M, D, TFSI)	0.252	2	(MW, D, Poly)	0.213	2
(MW, TFSI, TN)	0.250	2	(MW, D, TFSI)	0.163	2
(M, TFSI, Li)	0.211	2	(Li, TN, Cond)	0.124	2
(MW, TFSI, Cond)	0.196	2	(MW, TFSI, Li)	0.111	2
(MW, Li, Cond)	0.169	2	(Li, Poly, Cond)	0.095	2

Ranked winding (TFSI, Li Diffusivity, Conductivity)

Winding Numbers as Flexibility



Winding histogram w/outliers

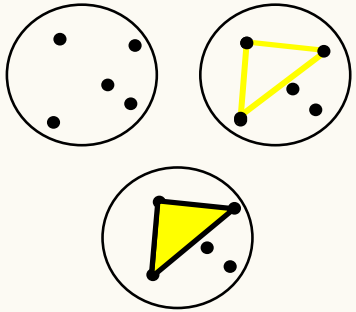
LOCAL PATHING

Open Questions and Potential Directions

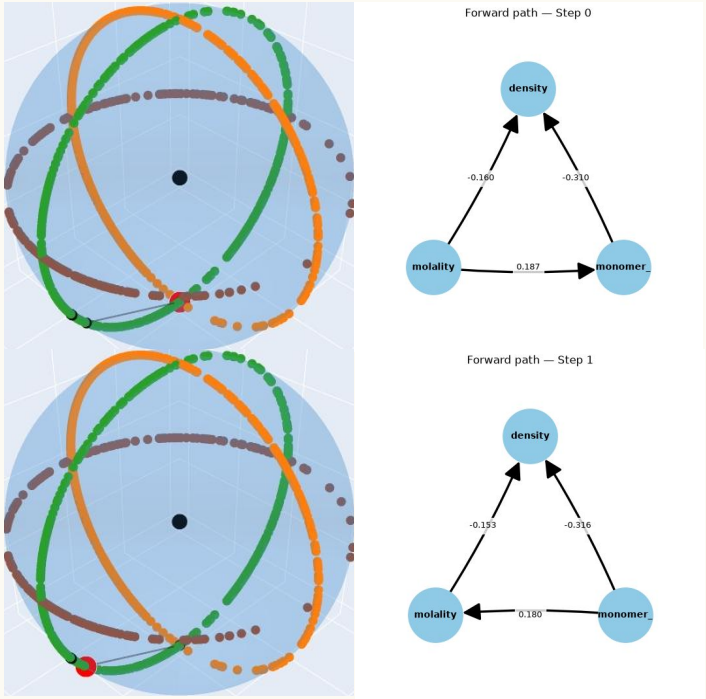
Higher Homology

Q: What are the higher homology groups of the link complex?
Q: How does data fill that space?

Quillen Fiber Approach
Persistent Homology on Smaller Cells

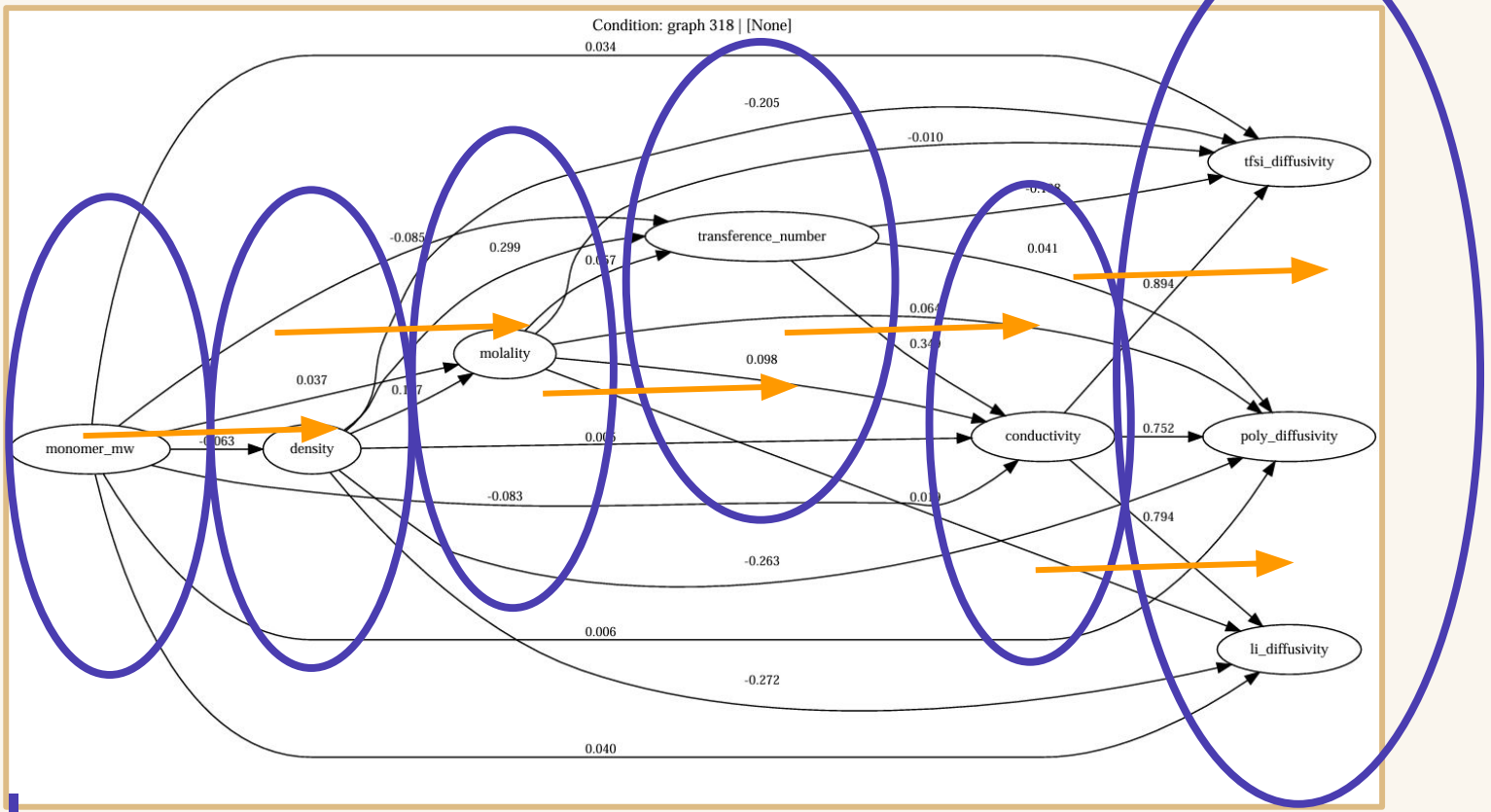


Better Winding Detection



CAUSAL REGIMES

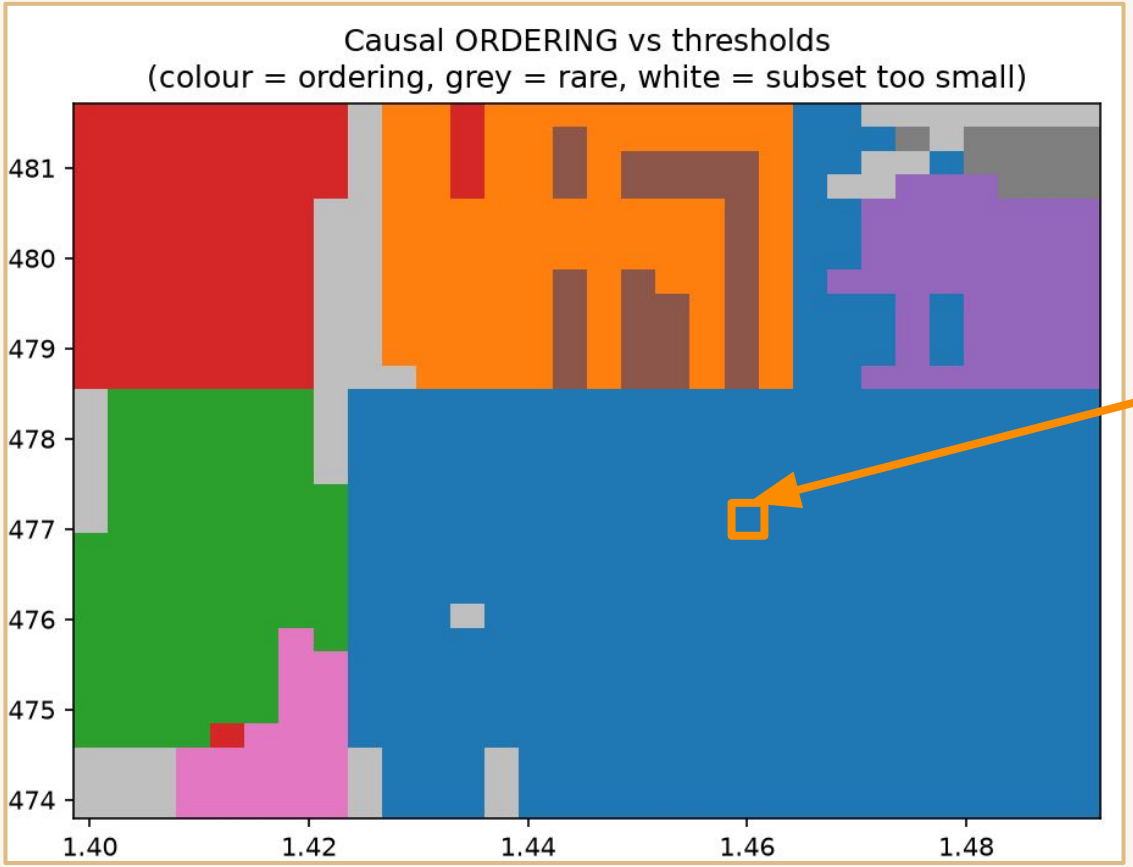
Topological Ordering



Question: When does causal ordering **change?**

CAUSAL REGIMES

Color by Topological Ordering



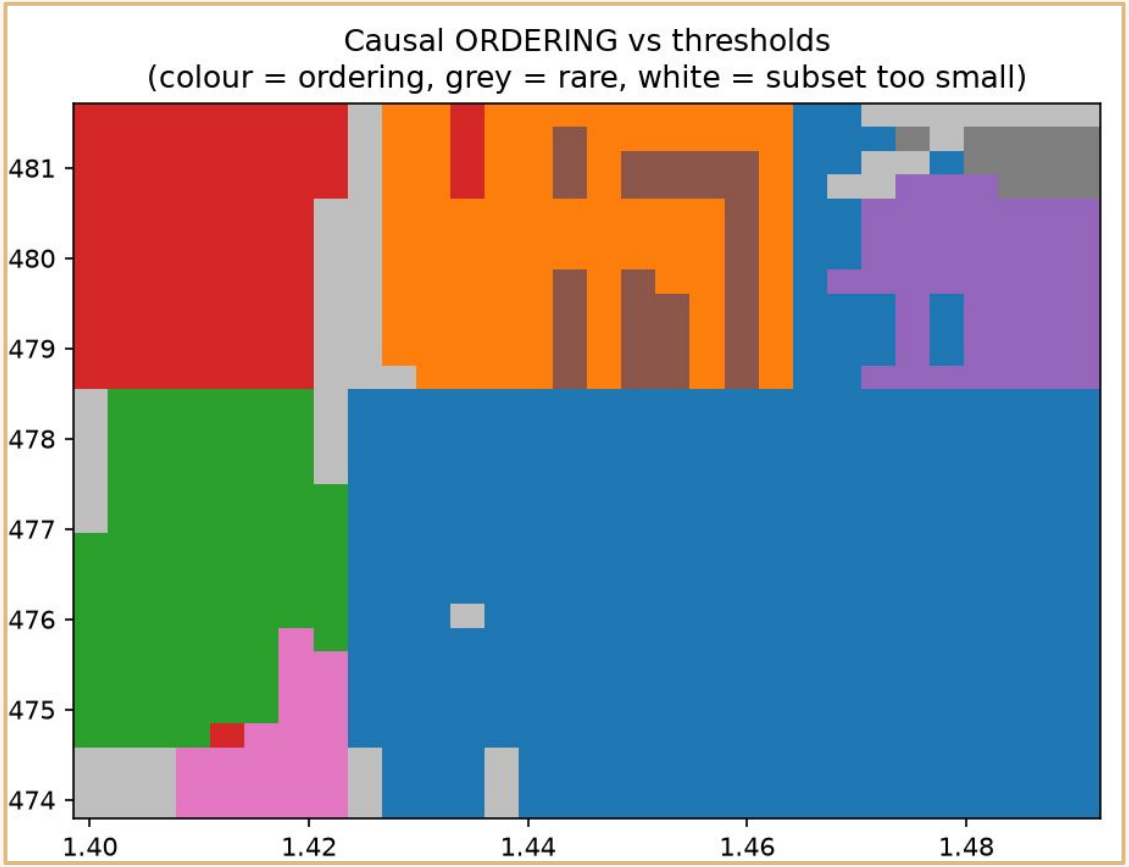
X axis : Molality < X
Y axis: monomer_mw < Y

Ex: Molality < 1.46 and monomer_mw < 477

Color = Topological Ordering

CAUSAL REGIMES

Color by Topological Ordering



Regions are **Causal Regimes**.

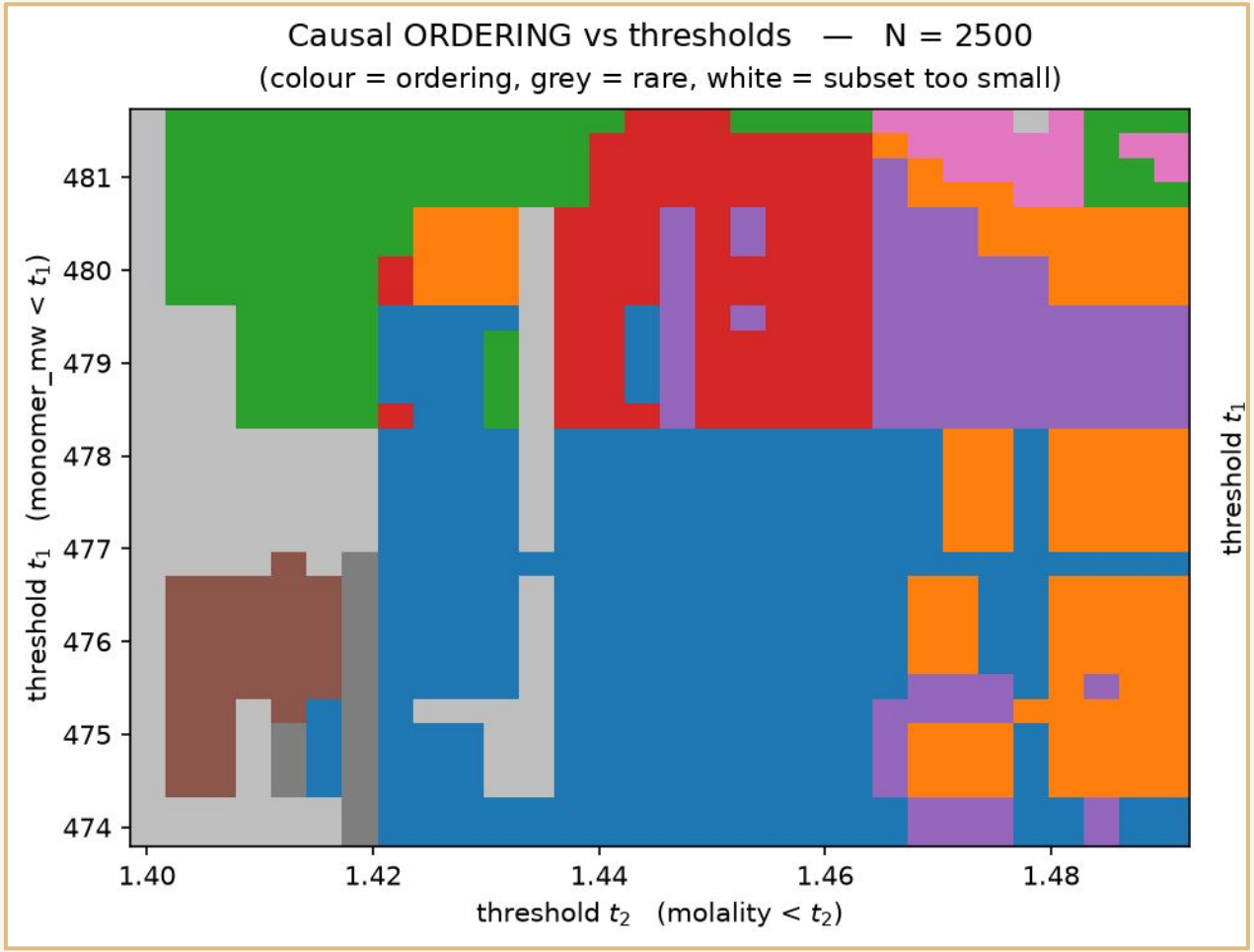
Boundaries are **potential discoveries**

CAUSAL REGIMES

Topological Orders

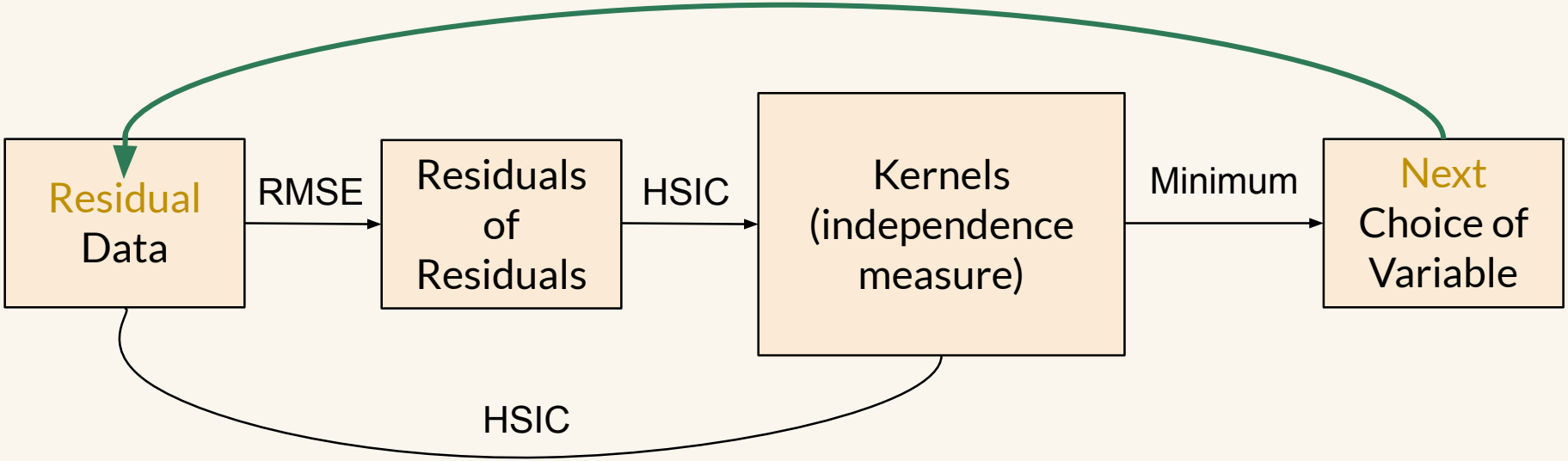
Convergence to **causal regimes**.
Convergence is **convincing**

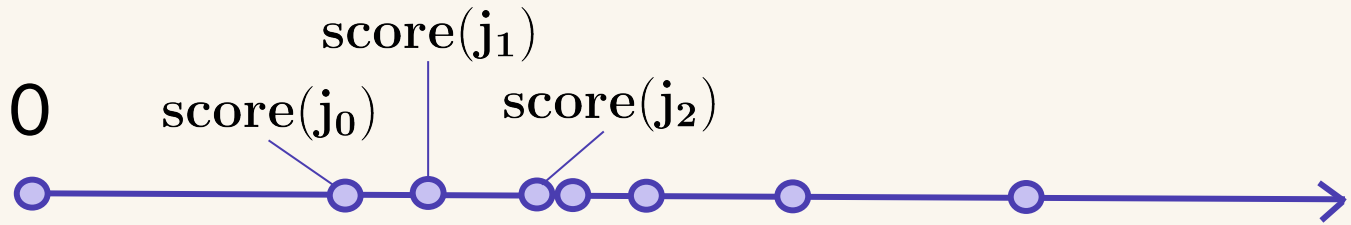
Only **two** of **several** dimensions.
True geometry is complicated



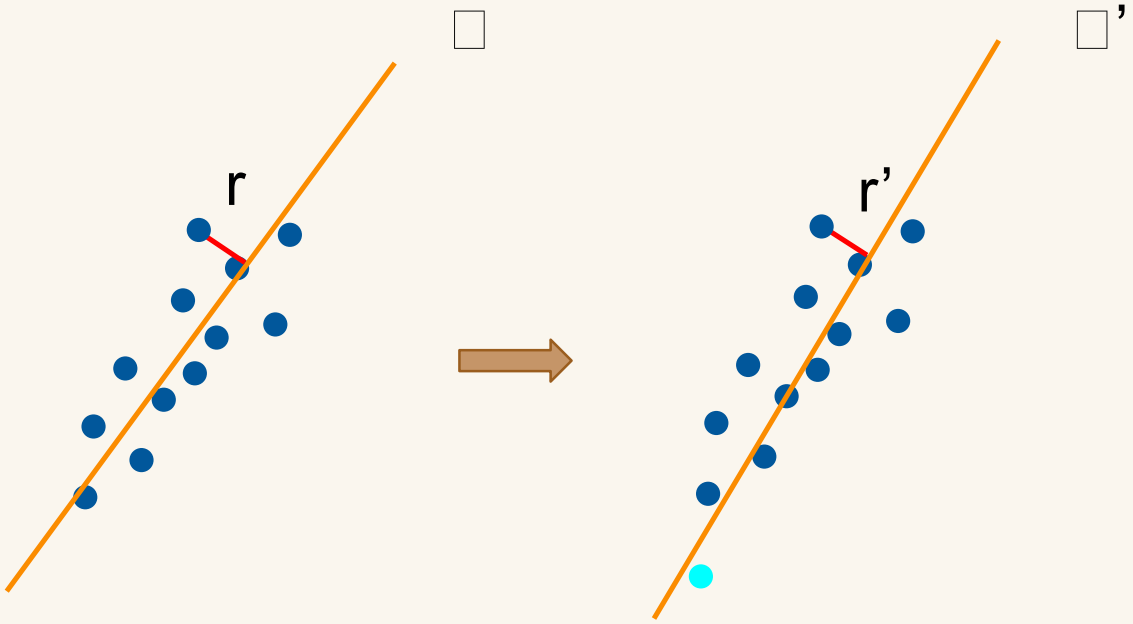
Causal Regimes as sample size increases

Direct LiNGAM Bound



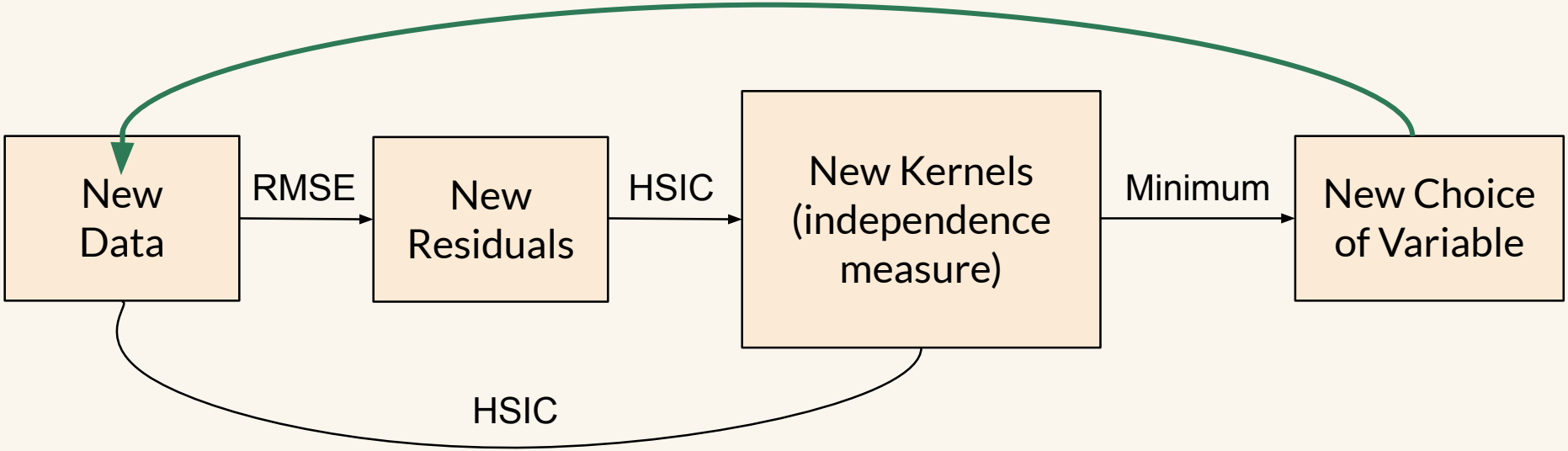


Direct LiNGAM Bound



Change by adding a new datapoint

Direct LiNGAM Bound



Q: When old ordering = new ordering

A: We have a bound

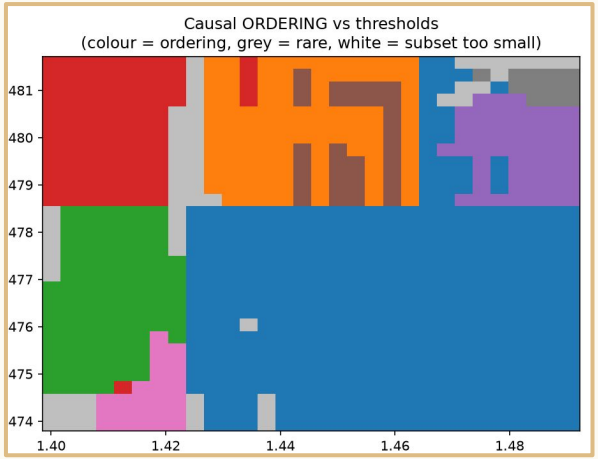
CAUSAL REGIMES

Future Work

Formalization condition space operations

For users and developers to approach discoverability.

Construct a formal way to measure dataset.



Theoretical Guarantees

Develop stability and rigid theory for convincingness.

Universal theory

Develop theory perfectly fits the assumption of DirectLiNGAM

TOPOLOGY OF CONDITIONAL CAUSALITY

Summary

Conditional Pathing

Highlight primary mechanism
Discoverability
Comprehensiveness <-> compute

Local Conditional Pathing

Substructure : discoverability
Winding number : convincingness

Topological Ordering

Change of causal order : discoverability

