Inferring Causal Relationships among Quantum States via Machine Learning

Omid Charrakh
Munich Center for Mathematical Philosophy

LMU Munich
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Motivation (1)

- Causal discovery algorithms (CDAs) are computational techniques for inferring causal relations among a set of variables from their statistical patterns.
- In classical (i.e., non-quantum) scenarios, it is possible to systematically achieve this goal thanks to the framework of the causal Bayes nets (CBNs).
- The same task cannot be straightforwardly accomplished in quantum mechanics (QM) because of some conflicts between the axioms of the CBN and QM.
- Some quantum physicists propose redefining the underlying axioms of the CBN in the quantum realm. This research program is called **quantum causal modeling**, or **quantum causality**.

Motivation (2)

- While there is no consensus on the precise formulation of quantum causal models, most present proposals require radical paradigm shifts surrounding fundamental notions of causation.

- Examples include redefining (Reichenbach's) principle of common cause, the causal Markov condition, the causal faithful condition, the notion of causal event, causal mechanism, intervention, acceptance of cyclic causal models, and indefinite causal orders.

- In contrast to the said research line, the present talk argues that most of the standard notions of causal modeling can be retained while still inferring causal relations among quantum systems from their statistical patterns.

- The key idea is to exploit machine learning (ML) to systematically extract hidden asymmetric patterns in the statistics of cause and effect.

Motivation (3)

- I will focus on a discovery algorithm called Randomized Causation Coefficient (RCC) and explain how to combine it with recent advances in ML (e.g., generative learning and active learning) to build a powerful causal learning algorithm for quantum systems.

- I will then present three simulated quantum scenarios and report the performance of this algorithm on them:
    1. cause **vs.** effect
    2. cause **vs.** effect **vs.** common cause **vs.** d-separation
    3. discovery in a multi-node network

- Finally, I will address some lessons and directions for extending this project.

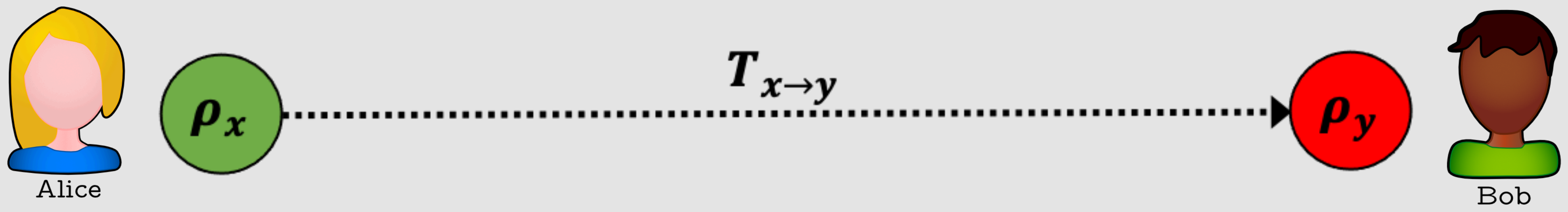
Contents

QM Scenario (1)

- Let Alice and Bob be two experimenters located in two labs, each having one qubit (i.e., the quantum version of a binary bit).

- Alice transmits the **quantum state** of her qubit to Bob. The state transmission is carried by a **quantum channel.**

- In QM, the quantum state is described by a 3-dim real vector called the **Bloch vector**, while the quantum channel is characterized by a set of matrices/operators.



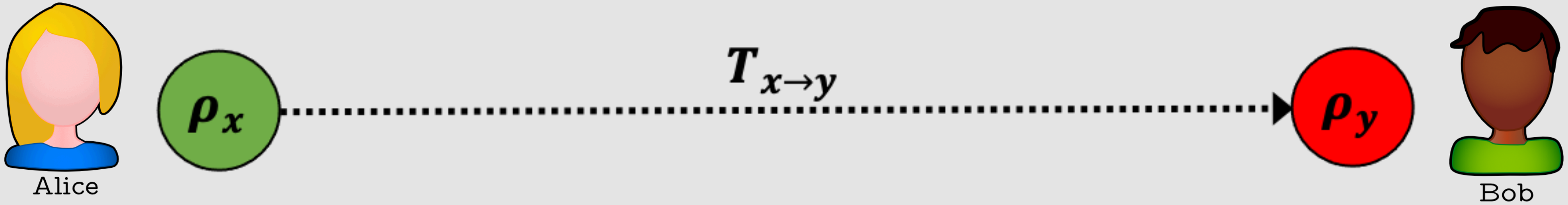
QM Scenario (2)

- In this scenario, there is an **asymmetry** arising from the directionality of the channel:

  A change in Alice's state might bring about a change in Bob's state. But <u>not the other way around</u>.

- Alice's state is the **cause**, and Bob's state is the **effect** $\Longrightarrow$ the channel direction is the causal direction.

- **Question:** Can we predict the causal direction merely from the qubits' states without explicitly performing interventions?

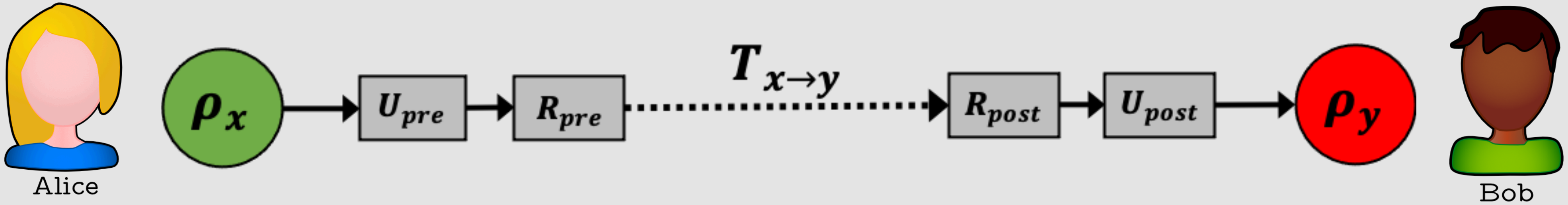


QM Scenario (3)

- Collaborating with Jan Dziewior from the Max Planck Institute of Quantum Optics, we simulated an experiment resembling this scenario.

- To make the simulation realistic, we add extra elements such as unitary operators, rotations, and noises to the channels.

- In our simplest simulation, we generate data sets containing the Bloch vectors of Alice and Bob as well as the causal direction.

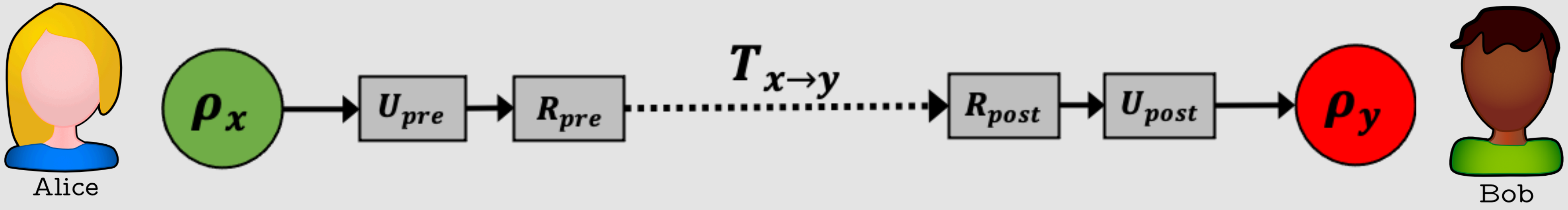


QM Scenario (4)

- Our **quantum channels** are probabilistic mixtures of the following six possibilities:

  - Identity
  - Dephase on $\boldsymbol{\sigma_z}$ basis
  - Dephase on a random basis
  - Replace by the pure state $\boldsymbol{\sigma_z^+}$
  - Replace by a random pure state
  - Replace by white noise

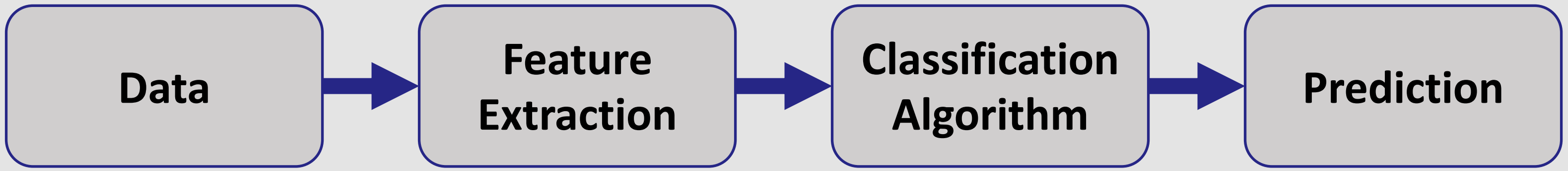
- Our noises take a Gaussian form but with random strengths.



RCC

- The RCC is a bivariate CDA that exploits ML to learn the causal direction between two random variables.

- The main idea of the RCC is to systematically extract the asymmetric features of cause and effect variables and train a classifier on top of the extracted features.



- The RCC needs many sample datasets whose causal directions are already known.

- The standard RCC is limited to 1-dim random variables (e.g., temperature vs. height) but I extended this idea to 3-dim random variables.

Scenario 1 (1)

- Our first (and simplest) scenario consists of only two parties (e.g., Alice and Bob), whose causal structure can be one of the two following possibilities:
  - **1** $\equiv$ X causes Y
  - **2** $\equiv$ Y causes X

- We generate $\mathbf{N_s} = \mathbf{5000}$ sample datasets, each with one set of physical parameters.

- Each sample contains $\mathbf{N_p} = \mathbf{1000}$ data points containing the Bloch vectors of Alice and Bob as well as the causal direction.

ρ_x	ρ_y	*label*

$, \cdots ,$

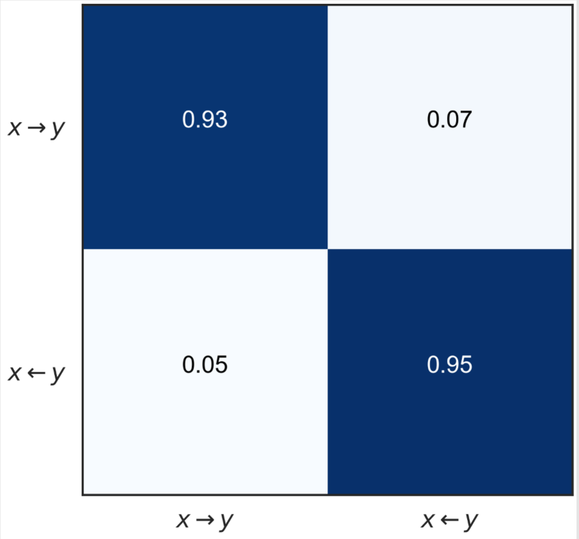
ρ_x	ρ_y	*label*

Scenario 1 (2)

- The samples are split into three subsets: 1) Training, 2) Validation, and 3) Test.

- After training the RCC classifier on the training set, the algorithm can predict the causal direction of other scenarios (with different physical parameters) from the Bloch vectors of the two labs.

- We got an accuracy of 94,5% on the test samples.



Scenario 2 (1)

➢ The second scenario also consists of only two parties, but this time the causal structure can be one of the four following possibilities:

- **0** $\equiv$ X and Y are causally independent
- **1** $\equiv$ X causes Y
- **2** $\equiv$ Y causes X
- **3** $\equiv$ X and Y are affected by a hidden common cause

➢ We again generate $\mathbf{N_s = 5000}$ sample datasets with $\mathbf{N_p = 1000}$ data points and train the RCC to distinguish four classes from the states of X and Y (Z is hidden).

ρ_x	ρ_y	*label*

, . . . ,

ρ_x	ρ_y	*label*

Scenario 2 (2)

➢ This time, we got an overall accuracy of 85,75% on the test samples.

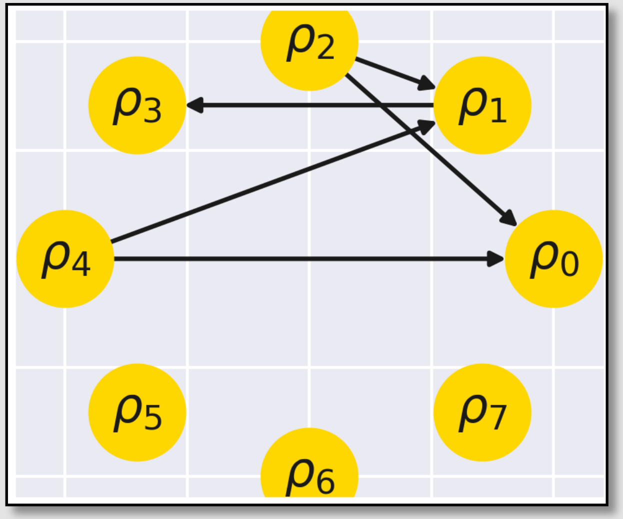
	$x \perp\!\!\!\perp y$	$x \rightarrow y$	$x \leftarrow y$	$x \leftarrow z \rightarrow y$
$x \perp\!\!\!\perp y$	0.89	0.08	0.03	0.00
$x \rightarrow y$	0.07	0.90	0.00	0.02
$x \leftarrow y$	0.12	0.02	0.80	0.06
$x \leftarrow z \rightarrow y$	0.00	0.10	0.06	0.84

Scenario 3 (1)

- The third scenario deals with a multi-node network where experimenters in different labs transmit their quantum states to other labs via pre-defined causal structures.

- The task is to predict the whole causal structure from the Bloch vectors of labs.

ρ_1	ρ_2	ρ_3	ρ_4	ρ_5	ρ_6	ρ_7	ρ_8



Scenario 3 (2)

- As the number of possible causal structures super-exponentially grows with the number of nodes, it would be naïve to define the classification classes in accordance with the number of possible causal graphs.

- Instead, we can focus on each pair of nodes and characterize their causal relation as one of the following three possibilities:

  - **0** $\equiv$ there is no causal edge between X and Y
  - **1** $\equiv$ there is a causal edge from X to Y
  - **2** $\equiv$ there is a causal edge from Y to X

- We consider $\mathbf{N_G = 230}$ graphs and split them into 1) Training, 2) Validation, and 3) Test graphs. For each graph, we generate $\mathbf{N_p = 1000}$ data points.

Scenario 3 (3)

➢ To extract the asymmetric features of each pair of nodes, we act as follows:

ρ_1	ρ_2	ρ_3	ρ_4	ρ_5	ρ_6	ρ_7	ρ_8

$$\rho_1 \;\; \rho_2 \mid \rho_3 \quad \rho_1 \;\; \rho_3 \mid \rho_2 \quad \rho_1 \;\; \rho_4 \mid \rho_2$$

$$\rho_1 \;\; \rho_2 \mid \rho_4 \quad \rho_1 \;\; \rho_3 \mid \rho_4 \quad \rho_1 \;\; \rho_4 \mid \rho_3$$

$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$

$$\rho_1 \;\; \rho_2 \mid \rho_8 \quad \rho_1 \;\; \rho_3 \mid \rho_8 \quad \rho_1 \;\; \rho_4 \mid \rho_8$$

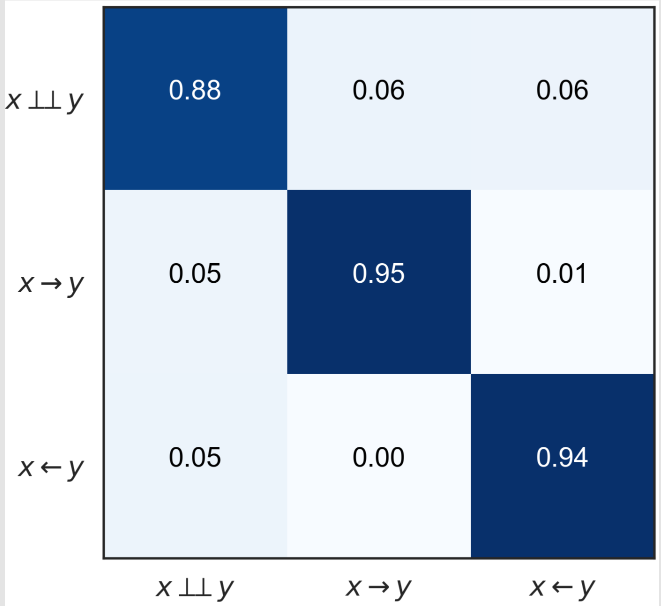
$$\boldsymbol{\mu}(P_S) = \Big(\mu(\rho_x),\;\; \mu(\rho_y),\;\; \mu(\rho_{xyz})\Big) \in \mathbb{R}^{3f}$$

Scenario 3 (4)

- Our complete ML pipeline encompasses many technical details, so I present the final results first. If time allows, I will also sketch some other details.

- In a multi-node scenario, the CDA performance can be examined at two levels:

  - **Local:** accuracy of predicted labels for node-pairs
  - **Global:** accuracy of the whole predicted graph

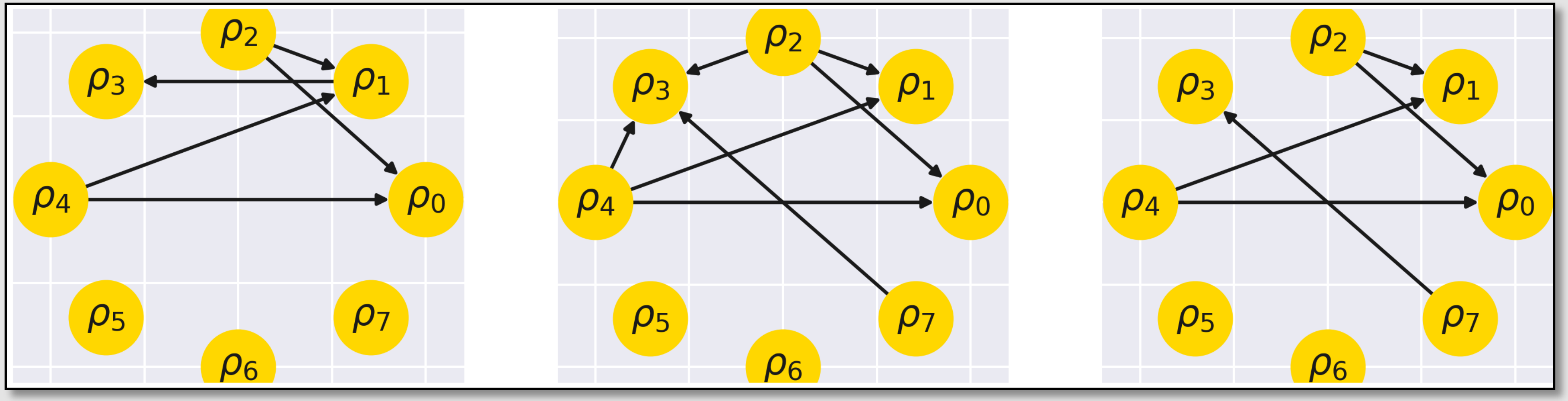


Scenario 3 (5)

- At the local level, we got an accuracy of 92,3% on the test samples.

- At the global level, we got **2,34** misclassified edges (averaged on 500 test graphs).

- Example:



True Graph | **Predicted Graph (raw)** | **Predicated Graph (post-processed)**

Pipeline

NN-simulator

Fit a regression model on the channel data from the mechanism graph
Simulate channel data via the NN-simulator for different causal graphs

Pre-process

Get all triples of 8-Nodes graphs from the original and simulated channel data
Featurize them
Pull them into one dataframe and store the causal directions as a separate column

Active Learning

Build a high-quality training dataset via Active Learning (AL)
Train a base classifier using initial and pool datasets

Re-Training

Take the dataset collected by the AL learner
Re-train and tune a more complex classifier on the AL data

Post-process

Confidence thresholding of the classifier
Edge penalization and pruning
Hill-climbing algorithm

Lessons & Future (1)

- ML enables the estimation of the causal direction among quantum systems from the statistical patterns these systems exhibit.

- A similar task can be accomplished by discovery algorithms developed in the context of quantum causal models.

- There are at least two advantages to using the ML approach compared to the latter:

1. *The ML approach is foundationally parsimonious*: it is inherently empirical and does not redefine the fundamental notions of causal modeling (e.g., the CBN axioms).

2. *The ML approach is empirically more efficient*: the starting point of quantum causal models is the reconstruction of the process matrix, which is empirically very complex and expensive. The ML approach does not need this complete information; it relies on local asymmetries between the node pairs.

Lessons & Future (2)

- Some directions for further research in this field:

1. Explain how ML can learn the causal direction. There should be some causal signature in the statistical data based on which a classifier predicts the causal direction. Can we physically interpret these signatures?

2. Extend the present model from the level of <u>states</u> to the level of <u>observables</u>. The current model compares the quantum states to estimate causal directions. In practice, one has measurement settings and outcomes rather than states.

3. Combine the present model with intervention-based CDAs. ML algorithms (e.g., reinforcement learning) can be helpful again. The example would be as follows. The algorithm provides the experimenters with instructions on efficient interventions/measurements revealing the whole causal structure of a scenario.

References

Lopez-Paz, David, et al. "Towards a learning theory of cause-effect inference." International Conference on Machine Learning. PMLR, 2015.

Goudet, Olivier, et al. "Learning functional causal models with generative neural networks." Explainable and interpretable models in computer vision and machine learning. Springer, Cham, 2018. 39-80.

Guyon, Isabelle, Alexander Statnikov, and Berna Bakir Batu, eds. Cause Effect Pairs in Machine Learning. Springer, 2019.

Peters, Jonas, Dominik Janzing, and Bernhard Schölkopf. Elements of causal inference: foundations and learning algorithms. The MIT Press, 2017.

Wood, C. J. & R. W. Spekkens (2012). The lesson of causal discovery algorithms for quantum correlations: Causal explanations of Bell-inequality violations require fine-tuning.

Oreshkov, Ognyan, Fabio Costa, and Časlav Brukner. "Quantum correlations with no causal order." Nature communications 3.1 (2012): 1-8.

Ried, Katja, et al. "A quantum advantage for inferring causal structure." Nature Physics 11.5 (2015): 414-420.

Allen, John-Mark A., et al. "Quantum common causes and quantum causal models." Physical Review X 7.3 (2017): 031021.

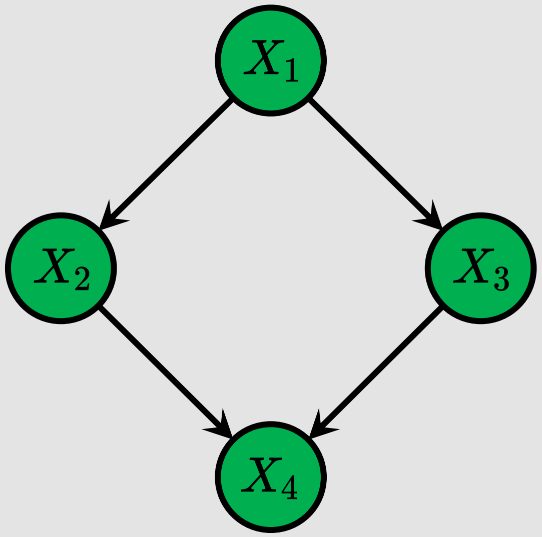
Costa, Fabio, and Sally Shrapnel. "Quantum causal modelling." New Journal of Physics 18.6 (2016): 063032.

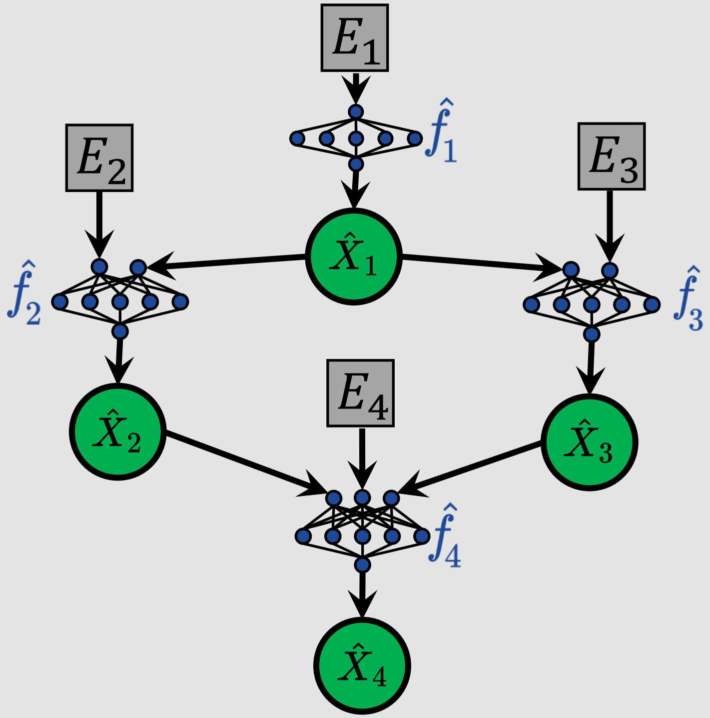
Giarmatzi, Christina. "A quantum causal discovery algorithm." Rethinking Causality in Quantum Mechanics. Springer, Cham, 2019. 125-150.

Barrett, Jonathan, Robin Lorenz, and Ognyan Oreshkov. "Cyclic quantum causal models." Nature communications 12.1 (2021): 1-15.

Supplementary Slides

NN Simulator



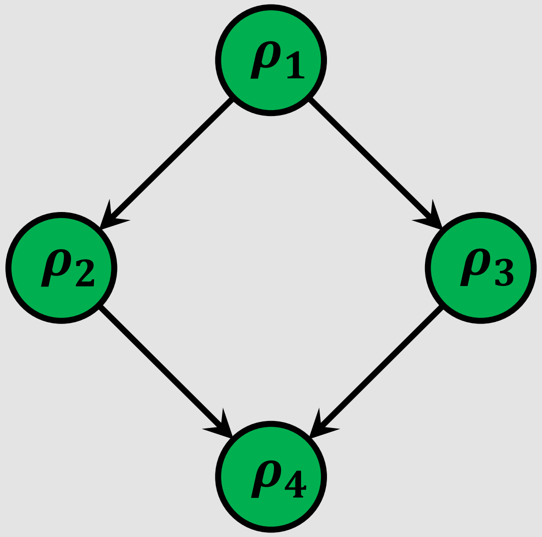


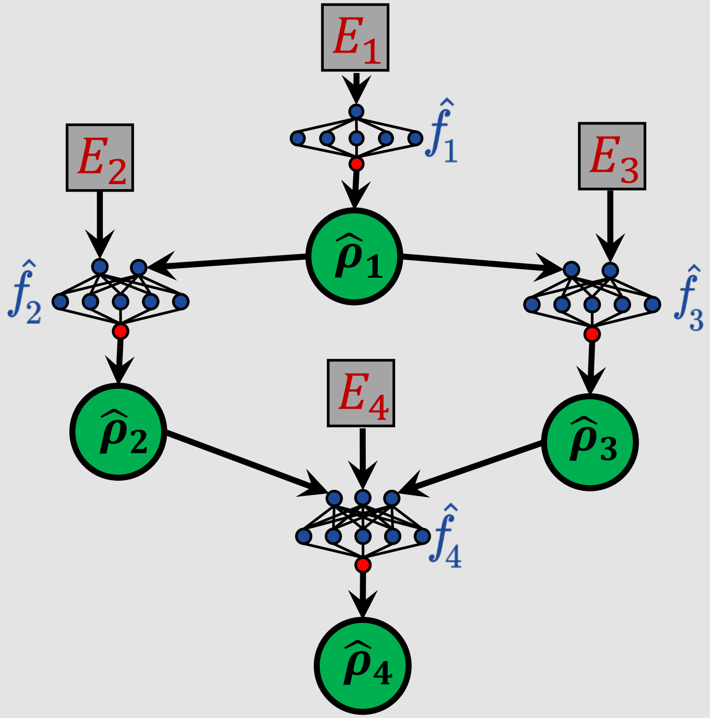
$$\begin{cases} \hat{X}_1 = \hat{f}_1(E_1) \\ \hat{X}_2 = \hat{f}_2\left(E_2, \hat{X}_1\right) \\ \hat{X}_3 = \hat{f}_3\left(E_3, \hat{X}_1\right) \\ \hat{X}_4 = \hat{f}_4\left(E_4, \hat{X}_2, \hat{X}_3\right) \end{cases}$$

- The Causal Generative Neural Networks (CGNN) is a generative CDA that exploits neural networks to estimate the underlying causal structure of a scenario.

- The standard version of the CGNN learns the causal mechanisms acting between classical 1-dim random variables => the NNs act as scalar-valued functions.

NN Simulator

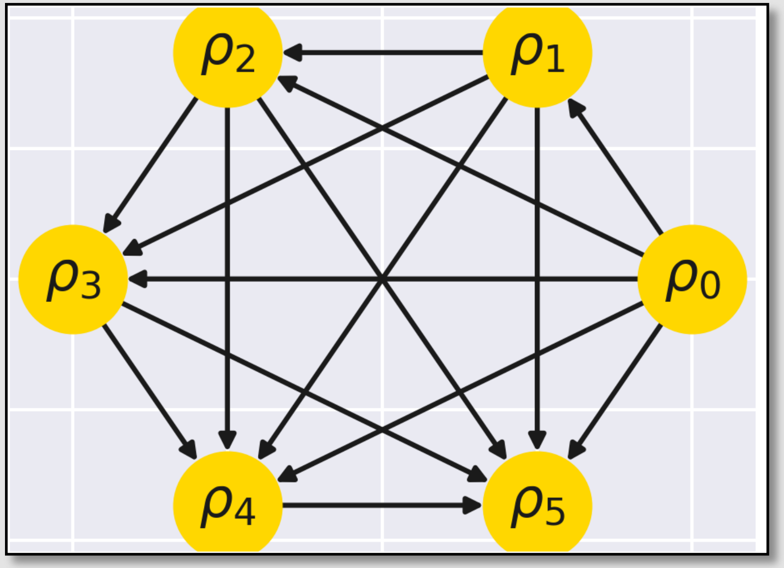


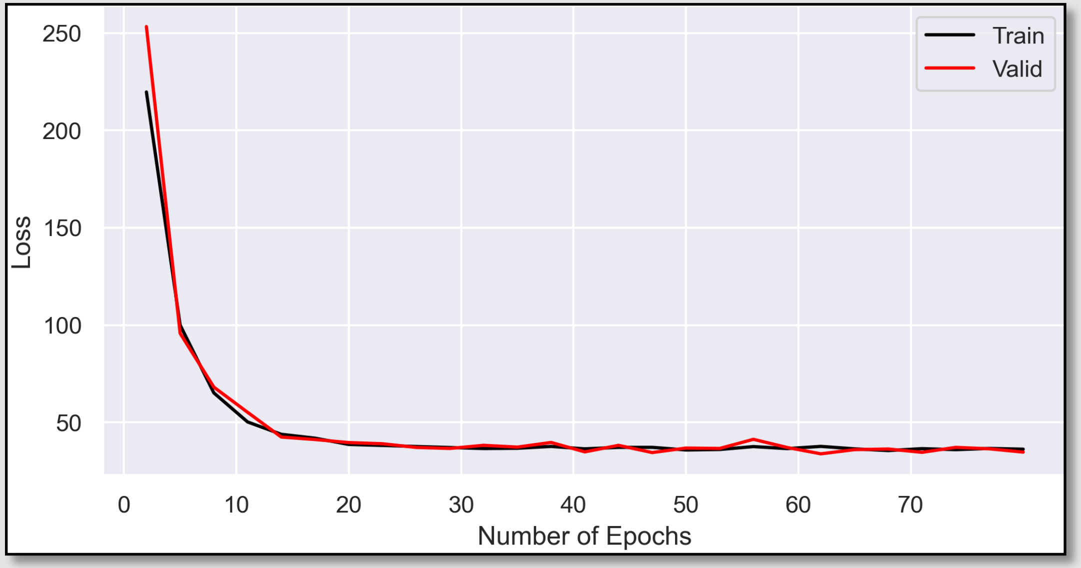


$$\begin{cases} \hat{\rho}_1 = \hat{f}_1(E_1) \\ \hat{\rho}_2 = \hat{f}_2(E_2, \hat{\rho}_1) \\ \hat{\rho}_3 = \hat{f}_3(E_3, \hat{\rho}_1) \\ \hat{\rho}_4 = \hat{f}_4(E_4, \hat{\rho}_2, \hat{\rho}_3) \end{cases}$$

- As a heuristic solution, I employed the CGNN to estimate the behavior of quantum channels.
- In my version, the noise variables and the NNs return 3 components, corresponding to the 3 components of Bloch vectors => the NNs act as vector-valued functions.

NN Simulator

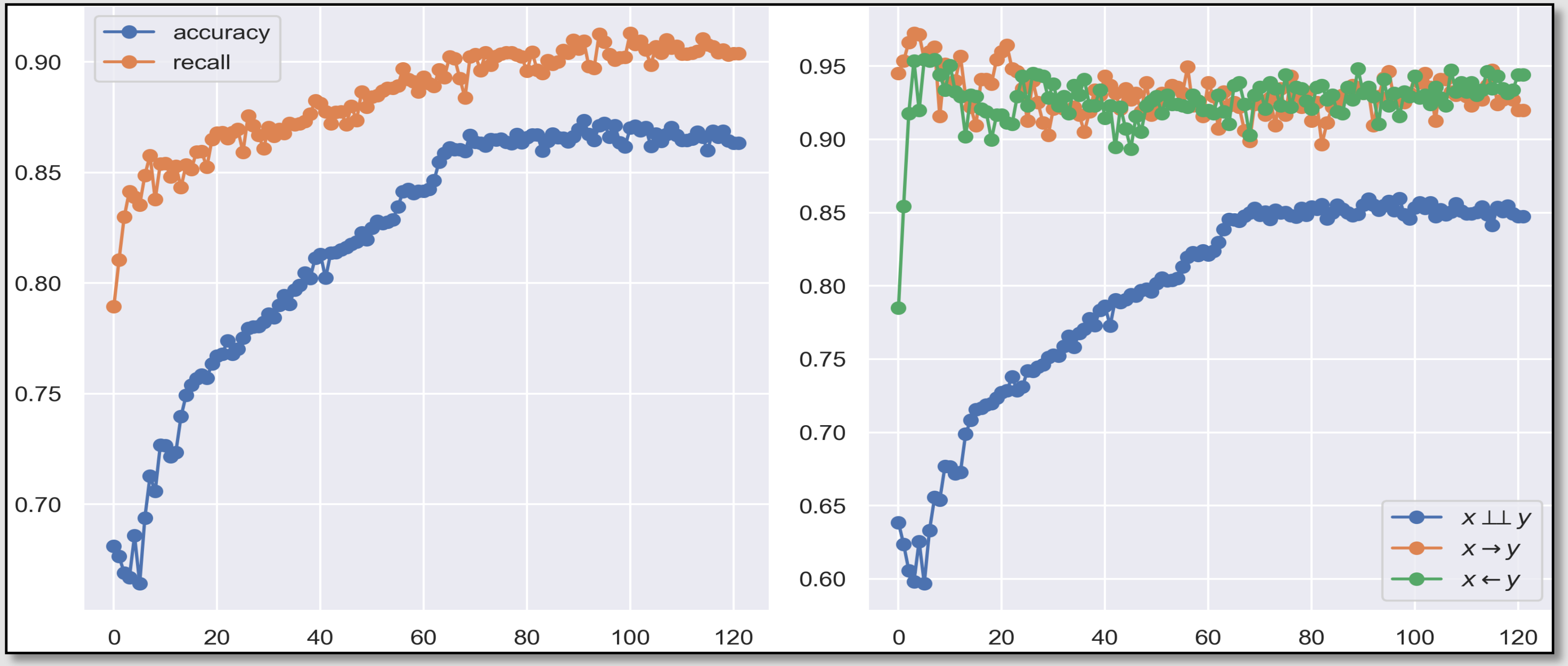




- To estimate the functional form of quantum channels, we fit a CGNN algorithm on the data from the causal graph shown above.

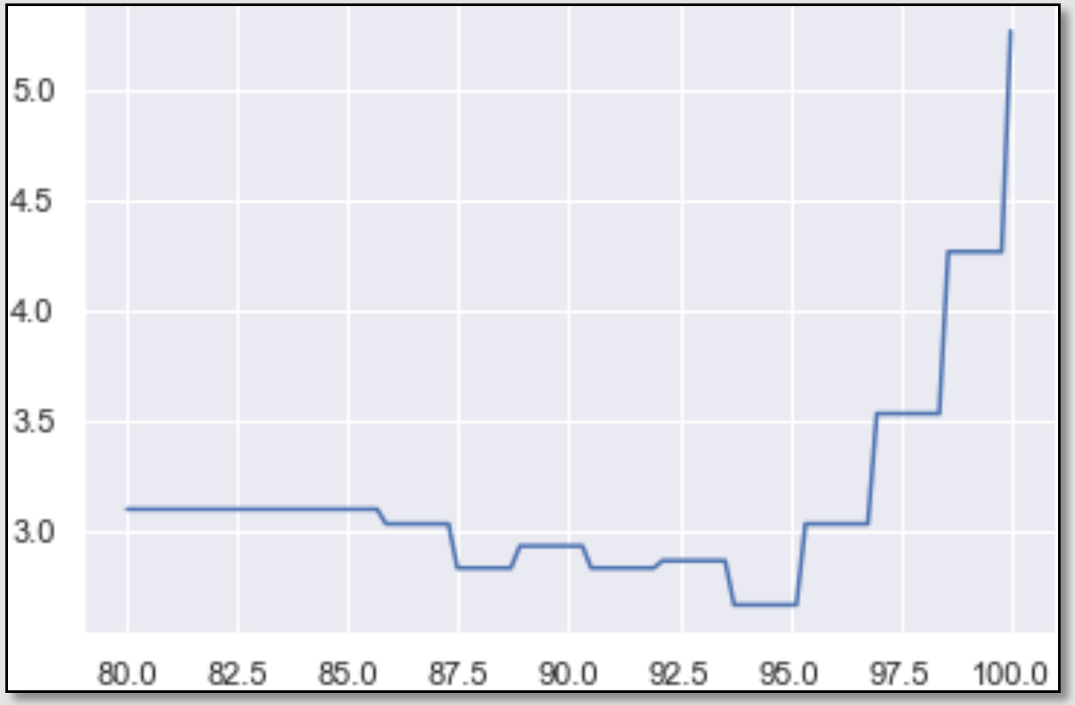
- This allows generating an arbitrary number of datasets for arbitrary causal structures.

Active Learning



- ➢ Active learning (AL) is a learning algorithm that can interactively query a user to label new data points with the desired outputs. By doing so, the machine can freely build its own training set.
- ➢ We use AL to build a high-quality training dataset, which is maximally informative and diverse.
- ➢ This strategy prevents the algorithm from overfitting.

Post-Processing



$$\mathcal{L} = \mathrm{MMD}(\mathscr{D}, \widehat{\mathscr{D}}) + \lambda|\widehat{\mathscr{G}}|$$

- We modify the raw predicted graph with three post-processing strategies:
  - confidence thresholding of the classifier
  - edge penalization and pruning
  - hill-climbing algorithm

RCC

- The feature extraction of RCC is based on the theory of Reproducing Kernel Hilbert Space (RKHS), where the featurization is done by embedding the empirical distributions of cause and effect variables:

$$\mu(\mathcal{Z}) = \frac{1}{N_p} \sum_{j=1}^{N_p} \left[\cos\left(w_1^\top z_j + b_1\right), \ldots, \cos\left(w_f^\top z_j + b_f\right)\right]^\top \in \mathbb{R}^f$$

$$\begin{cases} \mathcal{Z} = \{(z_j)\}_{j=1}^{N_p} \\ w_1, \ldots, w_f \in \mathbb{R}^d \\ b_1, \ldots, b_f \in \mathcal{U}(0, 2\pi) \in \mathbb{R}^1 \end{cases}$$

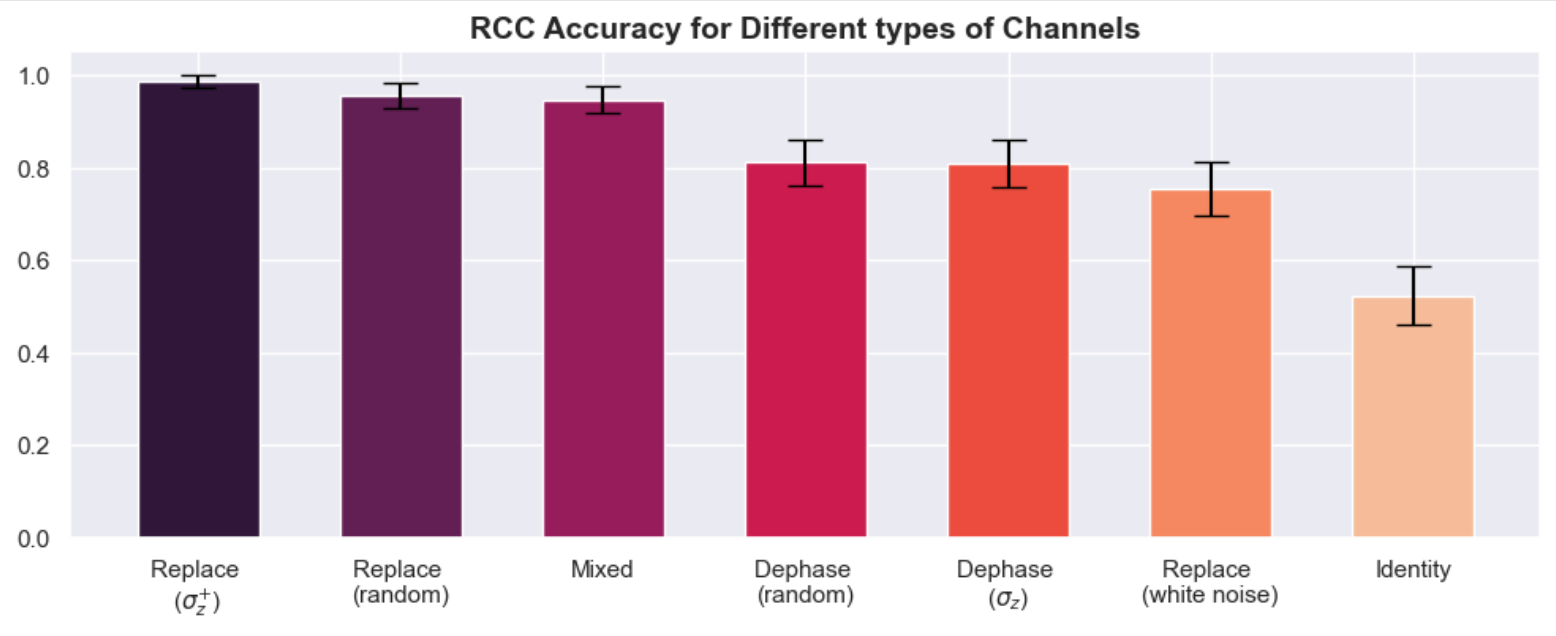
$$\boldsymbol{\mu}(P_S) = \Big(\underbrace{\mu(\rho_x)}_{\in \mathbb{R}^f}, \ \underbrace{\mu(\rho_y)}_{\in \mathbb{R}^f}, \ \underbrace{\mu(\rho_{xy})}_{\in \mathbb{R}^f} \Big) \in \mathbb{R}^{3f}$$

$$\boldsymbol{\mu}(P_S) = \Big(\mu(\rho_x), \ \mu(\rho_y), \ \mu(\rho_{xyz}) \Big) \in \mathbb{R}^{3f}$$

- The training dataset for the RCC classifier is obtained after featurization:

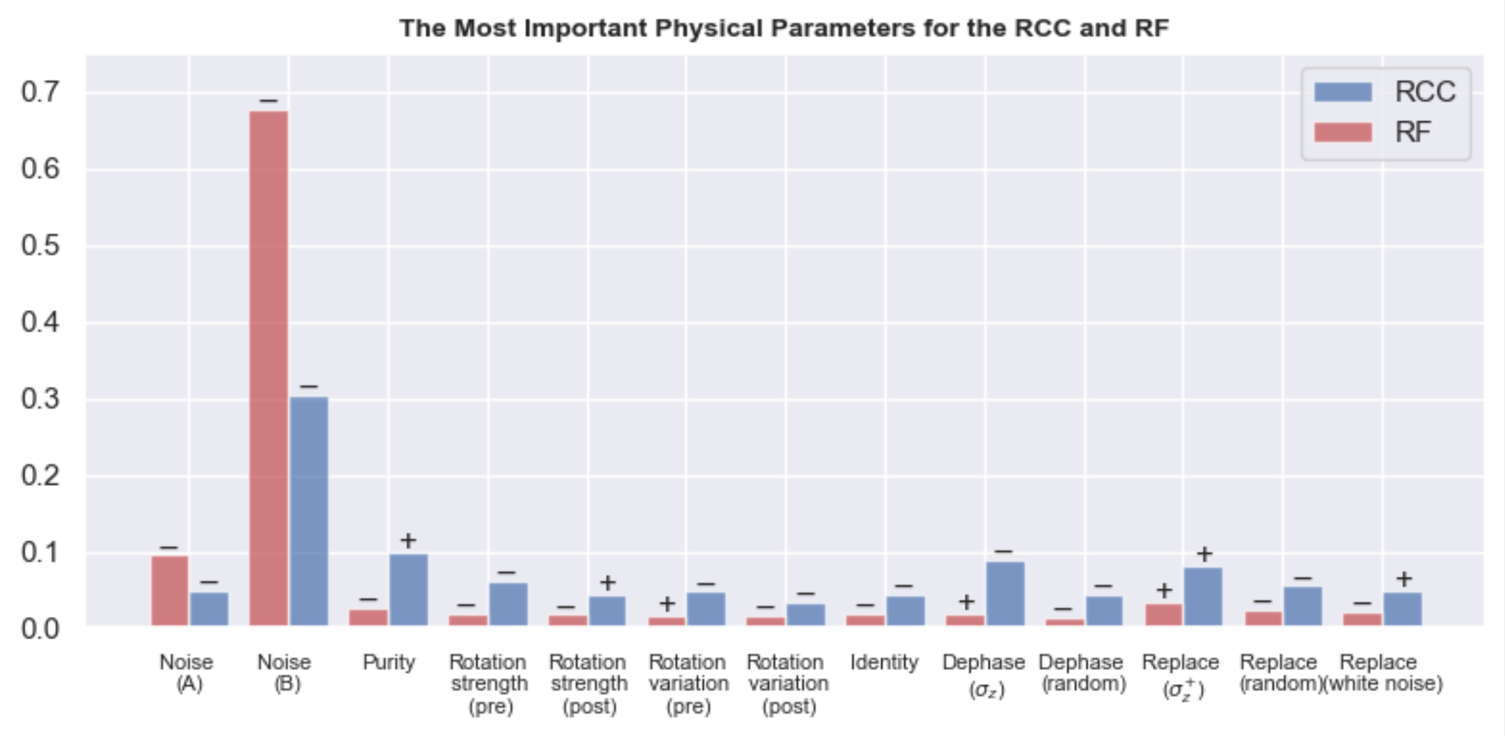
$$\text{Training Set} = \left\{(\boldsymbol{\mu}(P_{S_i}), l_i)\right\}_{i=1}^{N_s}, \ \text{where } l_i \in \{0, 1, 2\} \equiv \{\perp\!\!\!\perp, \rightarrow, \leftarrow\}$$

Scenario 1



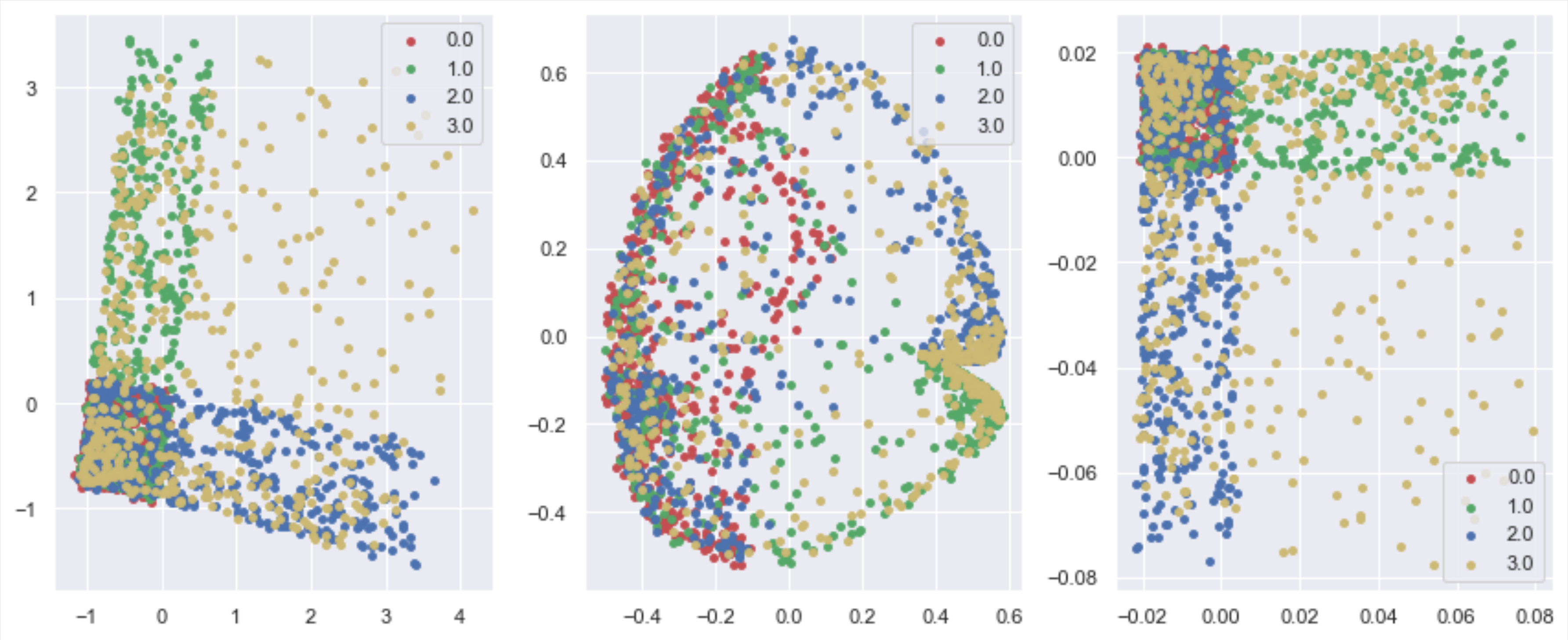
- To predict the causal direction, the RCC relies on asymmetric patterns in the statistics of cause and effect.
- If no asymmetry can be detected (or the asymmetry is very weak), the RCC can not distinguish cause from effect.
- This is the case for the “identity” quantum channel.

ML Black Box



- ➢ By comparing the performance of the RCC (as a causal learning algorithm) and a standard ML algorithm, we shed light on the black box of the RCC and examine the relationship between its performance and the physical parameters of each scenario.

PCA



- After the featurization of each dataset, a properly trained classifier must be to predict the corresponding label (i.e., causal direction) of that dataset.

- Figure above depicts how hard such a task is (datasets are mostly overlapped => hard to be distinguished by a human!).