A generalization of inversion using Bayes' rule

with applications to quantum

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Arthur Parzygnat (MIT)

more quantum

Based on:

① arxiv 2210.13531

Also published in Quantum

Joint w/ Francesco Buscemi (Nagoya University)

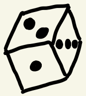
② arxiv: 2401.17447

more category theory

Non-commutative (quantum) inference?

Bayes' theorem and Bayesian inference is used ubiquitously for:

 Determining the disease of a patient based on symptoms and prior knowledge on the prevelance of diseases

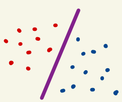
 Estimating the fairness of a die based on a few outcomes

 Determining future weather patterns based on previous ones

 Determining the state of a quantum system based on measurements and their outcomes

 Error-correction schemes

Betting on horse races or other probabilistic games

 Artificial intelligence, machine learning

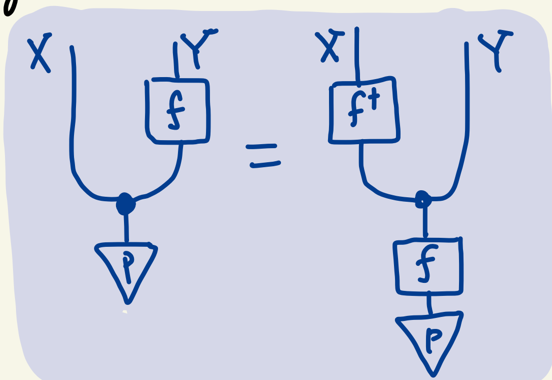
How can we make sense of quantum Bayes' theorem? Can we use it for quantum decision processes and inference?

Categorical & Quantum Bayesian inference

[Fong, Cho-Jacobs, Fritz]

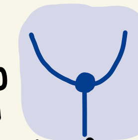
Given $I \xrightarrow{p} X$, $X \xrightarrow{f} Y$, a

Bayesian inverse is a $Y \xrightarrow{f^\dagger} X$ s.t.

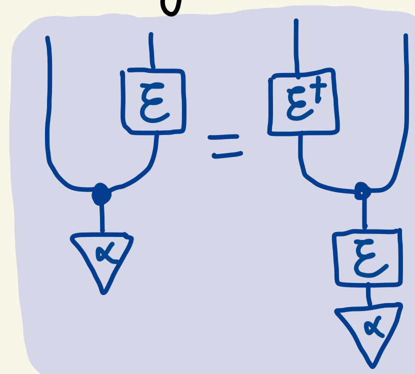


works quite well using Markov categories or classical categorical probability.

But...

the "copy" map  is not a valid operation (physical process) in quantum theory.

Furthermore, given $\mathbb{C} \xrightarrow{\alpha} A$, $A \xrightarrow{\mathcal{E}} B$, a Bayesian inverse $B \xrightarrow{\mathcal{E}^\dagger} A$ s.t.



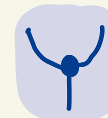
rarely exists...

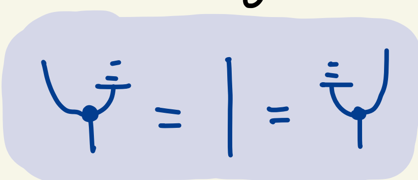
arXiv:2001.08375

arXiv:2005.03886 w/ Russo

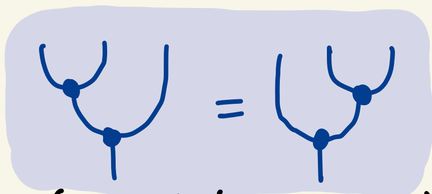
arXiv:2112.03129 w/ Giorgetti, Ranallo, & Russo

Markov categories

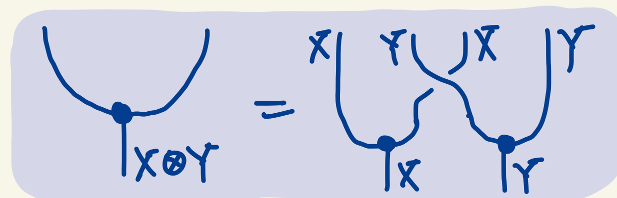
<u>Defn</u> A **Markov category** is a symmetric monoidal category where the monoidal unit is terminal and where each object X comes equipped with a **copy map** $X \to X \otimes X$  satisfying compatibility conditions such as

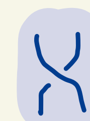


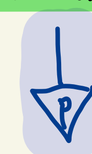
(broadcasting)

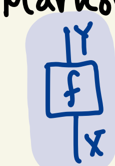


(associativity of Δ)



Here, $X \to I$  is called **grounding** and $X \otimes Y \to Y \otimes X$  the **braiding**.

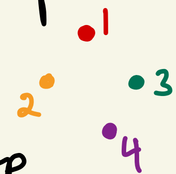
A **state** on X in a Markov category is a morphism $I \xrightarrow{p} X$ .

Morphisms $X \xrightarrow{f} Y$  are called **channels**.

Discrete probability FinStoch

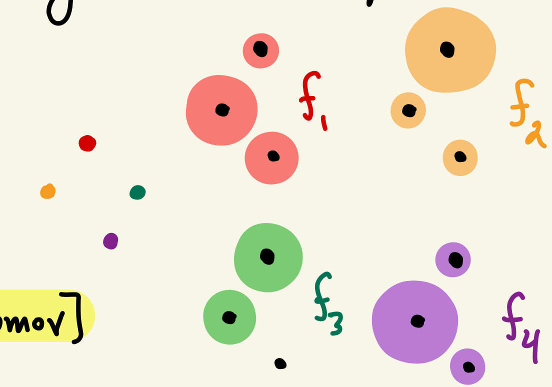
Discrete probabilities and conditional probabilities give an example.

object X finite set



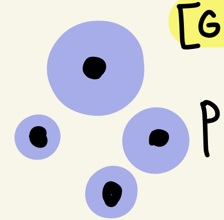
morphism $X \xrightarrow{f} Y$ stochastic map

- specifies probability f_x on Y for each $x \in X$
- gives probability f_{yx} at $y \in Y$



[Gromov]

state $I \xrightarrow{p} X$ probability on X



$X \otimes Y := X \times Y$ cartesian product

Note: In this talk, all states will be nowhere vanishing for simplicity.

$(f \otimes f')_{(y,y')(x,x')} = f_{yx} \times f'_{y'x'}$ product probabilities

Composition $(g \circ f)_{zx} = \sum_y g_{zy} f_{yx}$ Chapman-Kolmogorov (matrix multiplication)

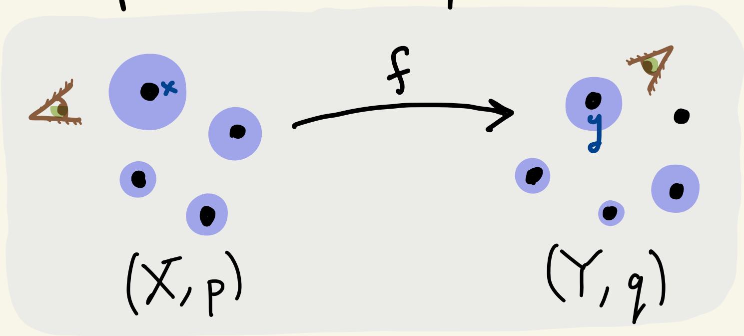
Stochastic maps push forward probabilities "belief propagation"

Category of classical states

CStates $\quad \mathrm{CStates} = I \downarrow \mathrm{FinStoch}$ coslice category

Objects: $(X, I \xrightarrow{p} X)$ General construction for any Markov category

Morphisms: $(X, p) \xrightarrow{f} (Y, q)$ so that $q = f \circ p$ "state-preserving"



prediction

$$q_y = \sum_x f_{yx}\, p_x$$

marginal likelihood $\quad$ likelihood $\quad$ prior

Composition: $(X, p) \xrightarrow{f} (Y, q) \xrightarrow{g} (Z, r) \quad (g \circ f)_{zx} = \sum_y g_{zy} f_{yx}$

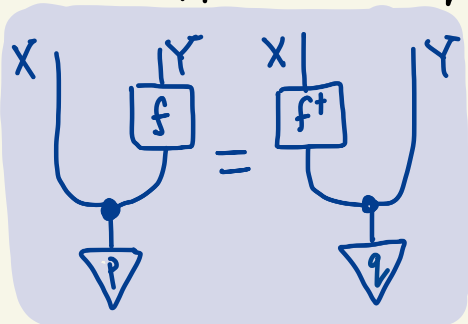
$\otimes$-product: $(X, p) \otimes (X', p') = (X \times X', p \otimes p')$

$(p \otimes p')_{(x,x')} = p_x p_{x'} \qquad (f \otimes f')_{(y,y')(x,x')} = f_{yx} f'_{y'x'}$

Markov Category Bayesian inverse

<u>Def'n</u> Given a Markov category C, a **Bayesian inverse** of a morphism $(X,p) \xrightarrow{f} (Y,q)$ in $I \downarrow C$ is a morphism $(X,p) \xleftarrow{f^\dagger} (Y,q)$

s.t.



Eg. $C = \mathrm{FinStoch}$ $\quad f^\dagger$ satisfies

$$f_{yx}\, p_x = f^\dagger_{xy}\, q_y \Rightarrow f^\dagger_{xy} = \frac{f_{yx}\, p_x}{q_y}$$

posterior

[Cho-Jacobs]

The Bayesian inverse is used for inference.

Given evidence y, $f^\dagger_{xy}$ gives the updated probability for x.

Eg.

Y	$p = 0.01$ disease	$1-p = 0.99$ ¬disease (X)	
positive test	0.9	0.05	} f_{yx}
negative test	0.1	0.95	

$q = 0.9 \times 0.01 + 0.05 \times 0.99 = 0.0585$

$1 - q = 0.9415$

Probability of having disease <u>given</u> positive test is $\bar{f}_{xy} = \frac{f_{yx}\, p_x}{q_y} \approx 0.154$

Bayesian inversion properties

Thm

$$\mathsf{CStates} \xrightarrow{\mathcal{R}} \mathsf{CStates}^{op}$$

$$(X,p) \xrightarrow{f} (Y,q) \longmapsto (X,p) \xleftarrow{f^\dagger} (Y,q)$$

$\mathcal{R}$ for retrodiction or reversal

defines an

identity-on-objects ($\mathcal{R}(X,p) = (X,p) \ \forall (X,p)$)

inverting ($\mathcal{R}(f) = f^{-1}$ whenever f^{-1} exists) ← does this have another name?

Note that f^{-1} must be stochastic which is guaranteed by def'n of the cats

involutive ($\mathcal{R}(\mathcal{R}(f)) = f \ \forall$ morphisms f)

monoidal ($\mathcal{R}(f \otimes f') = \mathcal{R}(f) \otimes \mathcal{R}(f') \ \forall$ morphisms f, f')

functor ($\mathcal{R}(id_{(X,p)}) = id_{(X,p)} \ \forall (X,p)$ and

$\mathcal{R}(g \circ f) = \mathcal{R}(f) \circ \mathcal{R}(g) \ \forall \ (X,p) \xrightarrow{f} (Y,q) \xrightarrow{g} (Z,r)$)

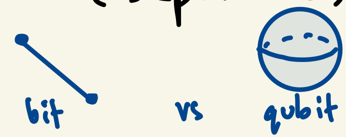
∴ CStates is a monoidal inverting dagger category! [Fritz]

Quantum extension?

Quantum states are positive unit-trace elements of f.d. C^*-algebras.
finite-dim'l

Eg. $\mathcal{A} = \mathcal{L}(\mathcal{H})$ bounded operators on Hilbert space $\mathcal{H}$ (separable)

pure state = rank 1 orthogonal projection



mixed state (density matrix) = self-adjoint operator w/ discrete spectrum forming a probability distribution

Eg. $\mathcal{H} = \mathbb{C}^m \Rightarrow \mathcal{A} \cong \mathbb{M}_m$ $m \times m$ matrices **(matrix algebra)**

Evolutions are **completely positive (CP) trace-preserving (TP)** maps, i.e.,

$\mathcal{A} \xrightarrow{\mathcal{E}} \mathcal{B}$ is **TP** iff $\mathrm{tr} \circ \mathcal{E} = \mathrm{tr}$ and **CP** iff $\mathrm{id}_{\mathbb{M}_m} \otimes \mathcal{E}$

is **positive** $\forall m \in \mathbb{Z}_+$, i.e., $\forall A\ \exists B$ s.t. $(\mathrm{id}_{\mathbb{M}_m} \otimes \mathcal{E})(A^*A) = B^*B$.

Such evolutions are also called **quantum channels**.

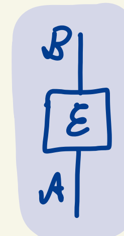
(CP condition guarantees a monoidal structure on evolutions)

A category of quantum states

QFinStoch

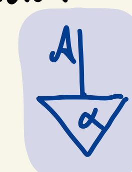
objects : f.d. C^*-algebras $\mathcal{A}$

morphisms : quantum channels $\mathcal{A} \xrightarrow{\mathcal{E}} \mathcal{B}$

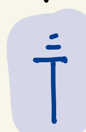


Composition: function composition $\otimes$ product as monoidal product

$\mathbb{C}$ as monoidal unit $\Rightarrow$ states given by $\mathbb{C} \xrightarrow{\alpha} \mathcal{A}$



$\mathbb{C}$ is still terminal



But NOT a Markov Category: no copy map!

No Cloning Theorem

QStates $= \mathbb{C} \downarrow$ QFinStoch still symmetric monoidal

objects : $(\mathcal{A}, \alpha)$

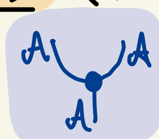
morphisms : $(\mathcal{A}, \alpha) \xrightarrow{\mathcal{E}} (\mathcal{B}, \beta)$ quantum channel s.t. $\mathcal{E}(\alpha) = \beta$

Semicartesian Categories

__Defn__ A **semicartesian category** is a symmetric monoidal category where the monoidal unit is terminal.

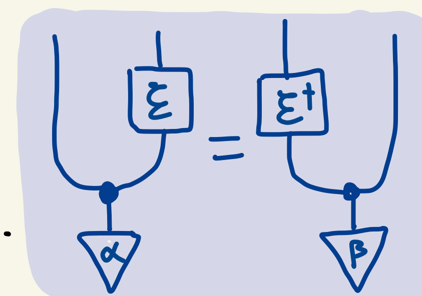
Eg. QFinStoch is semicartesian but not a Markov category. So how can we define Bayesian inversion in QStates?

__Attempt 1__ (Quantum Markov Categories arxiv: 2001.08375)

Define 

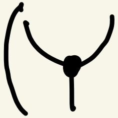
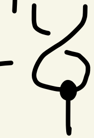
as the Hilbert-Schmidt adjoint of multiplication $\mathcal{A}\otimes\mathcal{A}\xrightarrow{\mu_{\mathcal{A}}}\mathcal{A}$ sending $A_1\otimes A_2$ to A_1A_2.

Although not positive, we can still define a Bayesian inverse of $(\mathcal{A},\alpha)\xrightarrow{\mathcal{E}}(\mathcal{B},\beta)$ via string diagrams and require $(\mathcal{A},\alpha)\xleftarrow{\mathcal{E}^{\dagger}}(\mathcal{B},\beta)$ to be a quantum channel.



Defining abstract retrodiction

"Problems" w/ Attempt 1

- $\mathcal{E}^{\dagger}$ is rarely a quantum channel ← may lack physical interpretation
- why not use  (multiplication in opposite order) or $\frac{1}{2}\Big($  $+$  $\Big)$?

↳ This leads to the subject of "quantum states over time"
arxiv: 2202.03607, 2212.08088 w/ Fullwood

Attempt 2 (semicartesian categories and daggers arXiv: 2401.17447)

Defn Let $\mathcal{C}$ be a semicartesian category w/ monoidal unit I, and let $\mathrm{States}(\mathcal{C}) = I \downarrow \mathcal{C}$ be its associated category of states. A retrodiction functor on $\mathrm{States}(\mathcal{C})$ is an identity on objects inverting involutive monoidal functor $\mathrm{States}(\mathcal{C}) \xrightarrow{\mathcal{R}} \mathrm{States}(\mathcal{C})^{op}$. Given $(A,\alpha) \xrightarrow{\mathcal{E}} (B,\beta)$, $(A,\alpha) \xleftarrow{\mathcal{R}(\mathcal{E})} (B,\beta)$ is the Bayesian inverse of $\mathcal{E}$.

Quantum retrodiction

Thm [P.-Buscemi] A retrodiction functor on QStates exists.

proof Given $(\mathcal{A},\alpha) \xrightarrow{\mathcal{E}} (\mathcal{B},\beta)$, the function $\mathcal{B} \xrightarrow{\mathcal{E}^{\dagger}} \mathcal{A}$ given by

$$\mathcal{E}^{\dagger}(B) := \sqrt{\alpha}\,\mathcal{E}^{*}\left(\frac{1}{\sqrt{\beta}}\,B\,\frac{1}{\sqrt{\beta}}\right)\sqrt{\alpha}$$

← called the **Petz recovery map**

statisfies all the conditions ∎

In this proof, $\mathcal{E}^{*}$ is the Hilbert–Schmidt adjoint of $\mathcal{E}$.

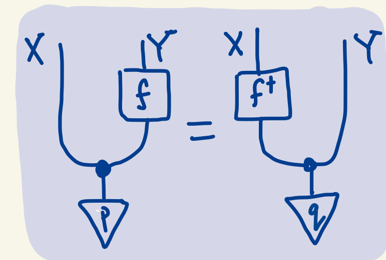
On commutative f.d. C^{*}-algebras, this reproduces classical Bayesian inversion (every commutative algebra $\mathcal{A}$ is of the form $\mathbb{C}^{X}$ for finite X and $\mathbb{C}^{X} \xrightarrow{\mathcal{E}} \mathbb{C}^{Y}$ corresponds uniquely to a stochastic map $X \xrightarrow{f} Y$).

Note: $\mathcal{E}^{\dagger}$ doesn't satisfy Cho-Jacobs defn but it still defines a dagger!

Also, functoriality of Petz is useful in quantum info! [Wilde arxiv:1505.04661]

Summary

- Markov categories provide a robust defn of Bayesian inversion via string diagrams.

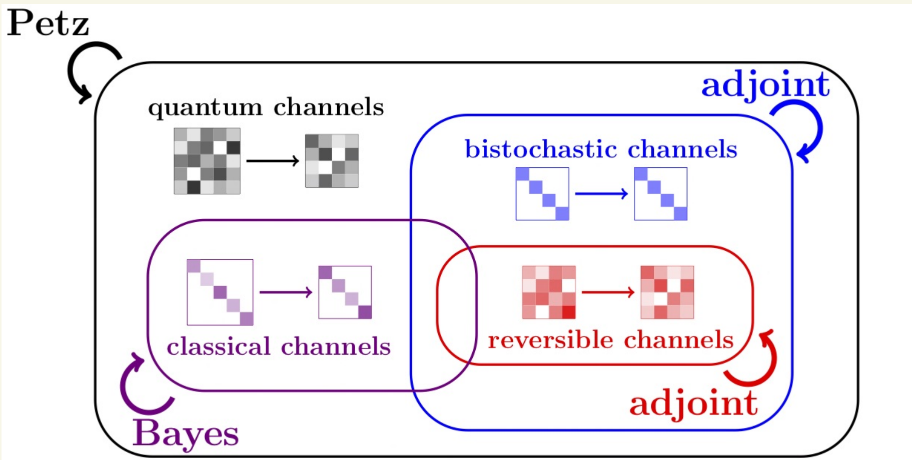


- However, this definition is somewhat limited when transferred to quantum systems and their evolutions.
- Key properties of the assignment sending $(X, p) \xrightarrow{f} (Y, q)$ to its Bayesian inverse are captured by retrodiction functors.
- Retrodiction functors can be defined on $I \downarrow C$ for any semicartesian category C.
- Bayesian inversion can be extended in a robust manner to quantum processes by viewing the latter as a semicartesian category.

So many questions

1. Is the classical Bayesian inversion the unique retrodiction functor $\mathsf{CStates} \longrightarrow \mathsf{CStates}^{op}$?
2. Is the Petz retrodiction the unique retrodiction functor $\mathsf{QStates} \longrightarrow \mathsf{QStates}^{op}$?
3. What structure/properties on a semicartesian category $\mathcal{C}$ guarantee the existence/uniqueness of a retrodiction functor $I \downarrow \mathcal{C} \longrightarrow (I \downarrow \mathcal{C})^{op}$?
4. What examples outside classical/quantum probability admit retrodiction functors and do they provide a useful way to "invert" morphisms?

Thank you!



arxiv: 2210.13531

Audience!

Collaborators

F. Buscemi
J. Fullwood
L. Giorgetti
A. Ranallo
B. Russo

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