Correlations, Cones and Cockroaches

(aka "Completely Positive Realisation Problem")

Andreas Winter (ICREA & Universitat Autònoma de Barcelona)

[with A. Monras, JMP 57:015219 (2016); arXiv:1412.3634]

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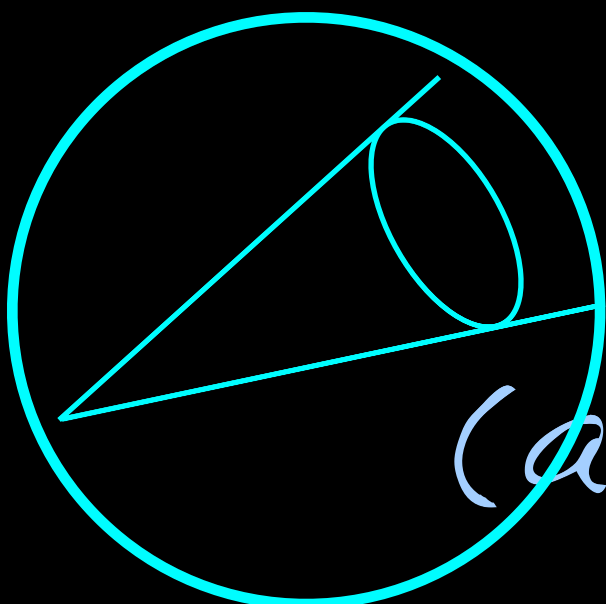
$P(uv\ldots w)$



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Basic question in inference/machine learning:

How to explain "large" data
with a "simple" model?

Concretely, observations are an infinite time series $\dots u_{-k} \dots u_{-1}\, u_0\, u_1\, u_2 \dots u_\ell \dots$

[$u_t \in \mathbb{M}$ letters from a finite alphabet].

Assume stationarity, i.e. for all t and ℓ,

$$P(u_1\, u_2 \dots u_\ell) = P(u_t\, u_{t+1} \dots u_{t+\ell-1}).$$

These marginals, for all finite words

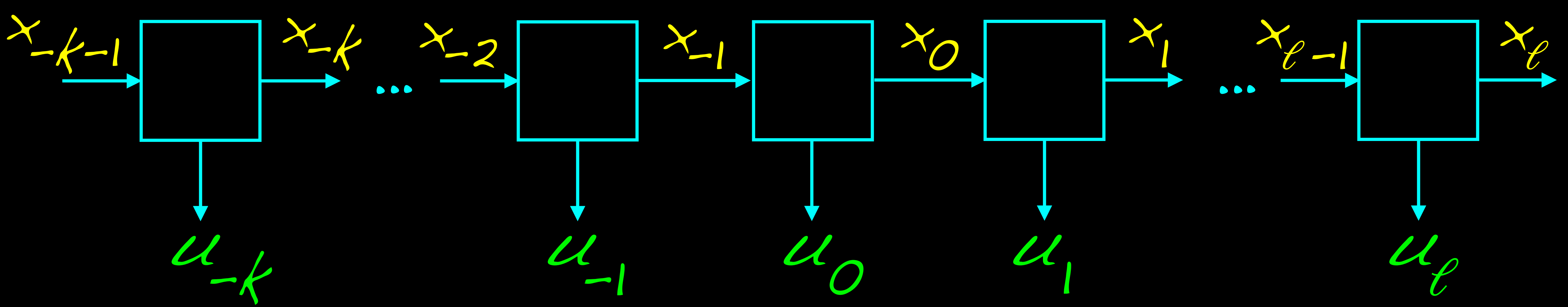
$$\underline{u} = u_1\, u_2 \dots u_\ell \in \mathbb{M}^* = \bigcup_{k \geq 0} \mathbb{M}^k,$$

determine the probability law.

Basic question in inference/machine learning:

How to explain "large" data with a "simple" model?

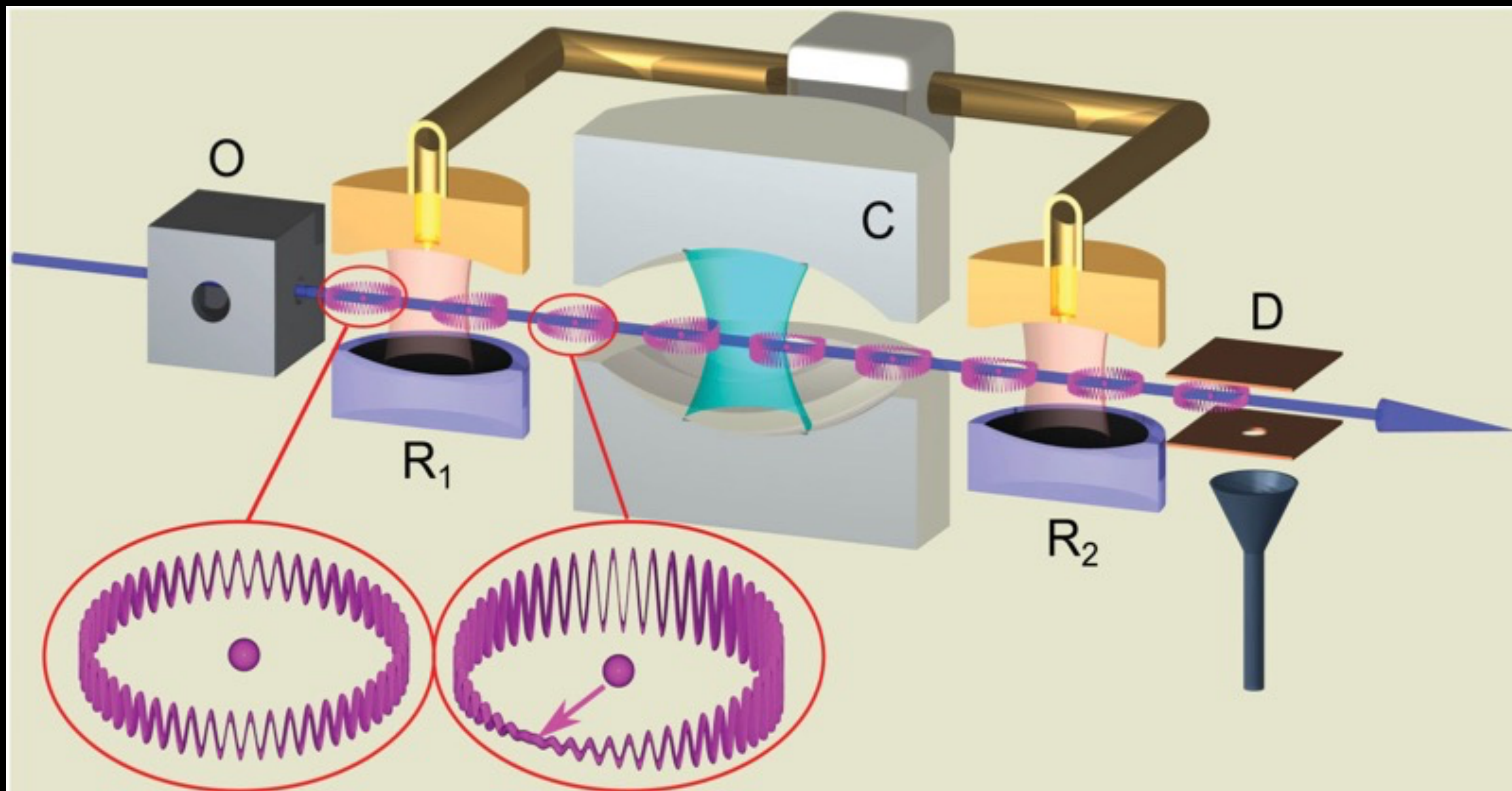
"Explanation" of $P(\underline{u})$ via a finite memory system as hidden cause:



Of course, need to specify the nature of the causation, and of the memory...

Example: Cavity-atom interaction

[S. Haroche, Physics Nobel Prize 2012]:

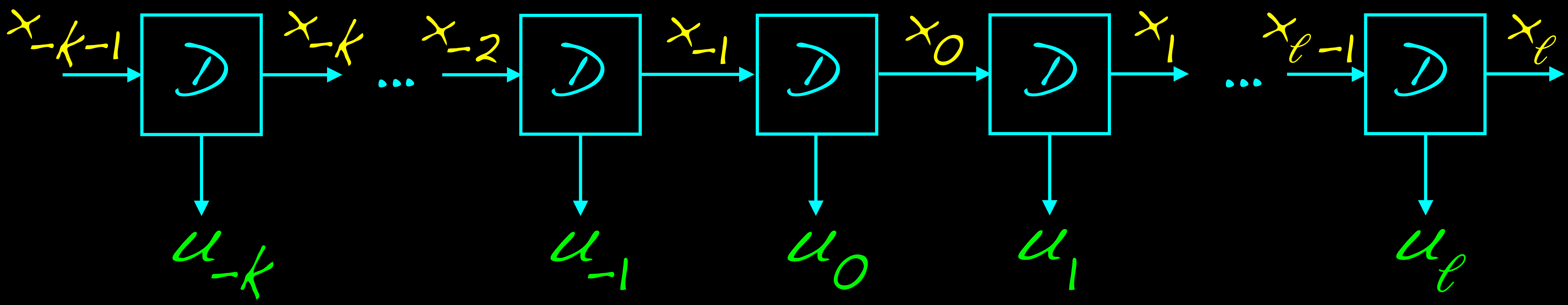


Outline

0. Observations as consequence of a finitary hidden cause (memory)
1. Classical, quantum and GPT memory
2. Reconstructing a quasi-realisation
3. On minimality, quotients & scarrafoni
4. How to reconstruct the positive cone?
5. Many questions...

I-a. Classical memory

The $x_t \in \mathbb{X}$ are from a finite set of internal states, $\mathcal{D} : \mathbb{X} \to \mathbb{X} \times \mathbb{M}$ are stochastic maps:



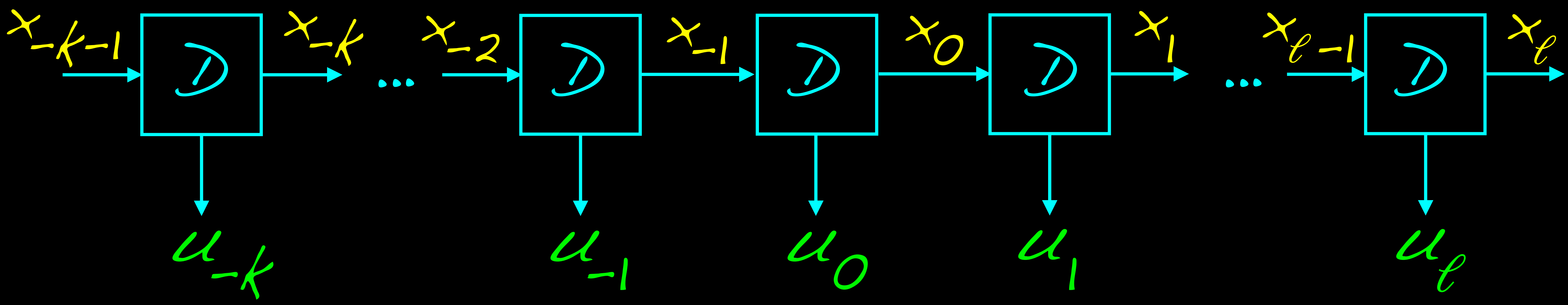
$\mathcal{D}_u : \mathbb{X} \to \mathbb{X}$ are sub-stochastic maps, s.t. $\overline{\mathcal{D}} = \sum_u \mathcal{D}_u$ is stochastic with stationary distribution π: $\overline{\mathcal{D}}\vec{\mathbf{1}} = \vec{\mathbf{1}}$, $\pi\overline{\mathcal{D}} = \pi$.

$$P(u_1 u_2 \ldots u_\ell) = \pi \mathcal{D}_{u_1} \mathcal{D}_{u_2} \cdots \mathcal{D}_{u_\ell} \vec{\mathbf{1}}$$

(c.r.)

1-6. Quantum memory

The $x_t \in \mathbb{X} = S(\mathcal{H})$ are quantum states on $\mathcal{H}$, and $\mathcal{D}$ is a completely positive instrument:



$\mathcal{D}_u : \mathbb{X} \to \mathbb{X}$ are completely positive maps, s.t. $\overline{\mathcal{D}} = \sum_u \mathcal{D}_u$ is unital (cpup) with stationary state ω: $\overline{\mathcal{D}}\mathbb{1} = \mathbb{1}$, $\omega \circ \overline{\mathcal{D}} = \omega$.

$$P(u_1 u_2 \ldots u_\ell) = \omega \circ \mathcal{D}_{u_1} \circ \mathcal{D}_{u_2} \cdots \circ \mathcal{D}_{u_\ell} \mathbb{1} \qquad \text{(c.p.r.)}$$

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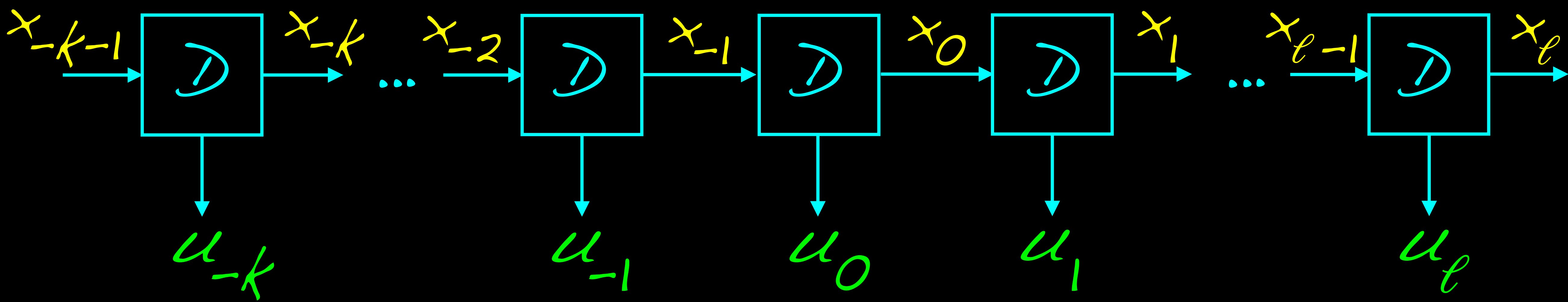

$\mathcal{D}_u : \mathbb{X} \to \mathbb{X}$ are completely positive maps, s.t.

$\overline{\mathcal{D}} = \sum_u \mathcal{D}_u$ is unital (cpup) w

state ω: $\overline{\mathcal{D}}\mathbb{1} = \mathbb{1}$, $\omega \circ \overline{\mathcal{D}} = \omega$.

Finitely correlated state (aka MPS)!

$$P(u_1 u_2 \ldots u_\ell) = \omega \circ \mathcal{D}_{u_1} \circ \mathcal{D}_{u_2} \cdots \circ \mathcal{D}_{u_\ell} \mathbb{1}$$

(c.p.r.)

1-6. Quantum memory

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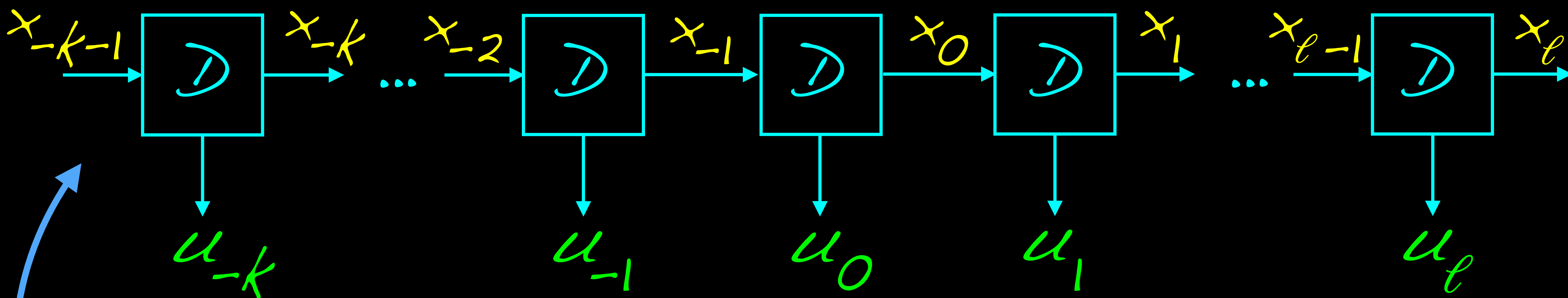
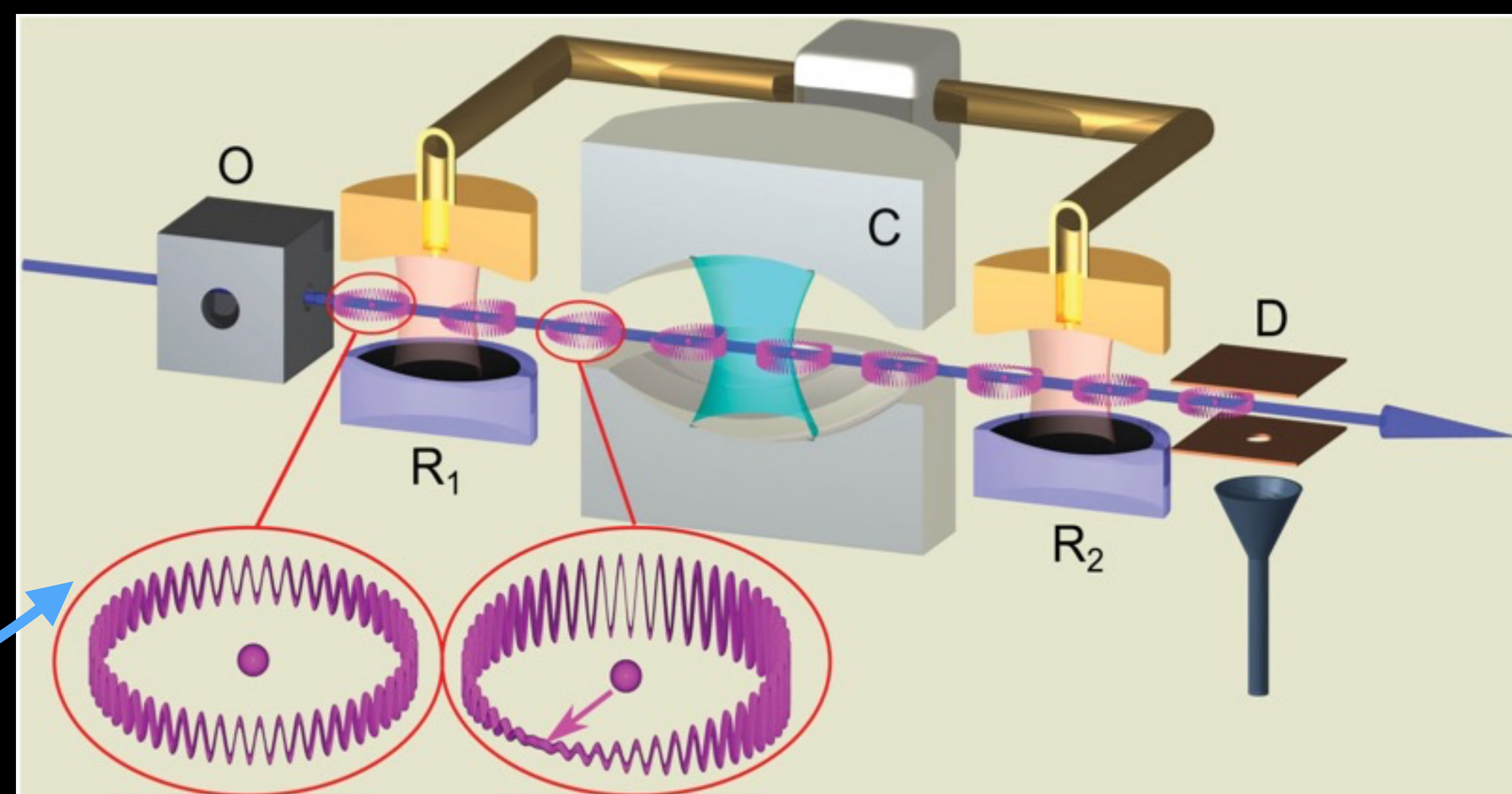
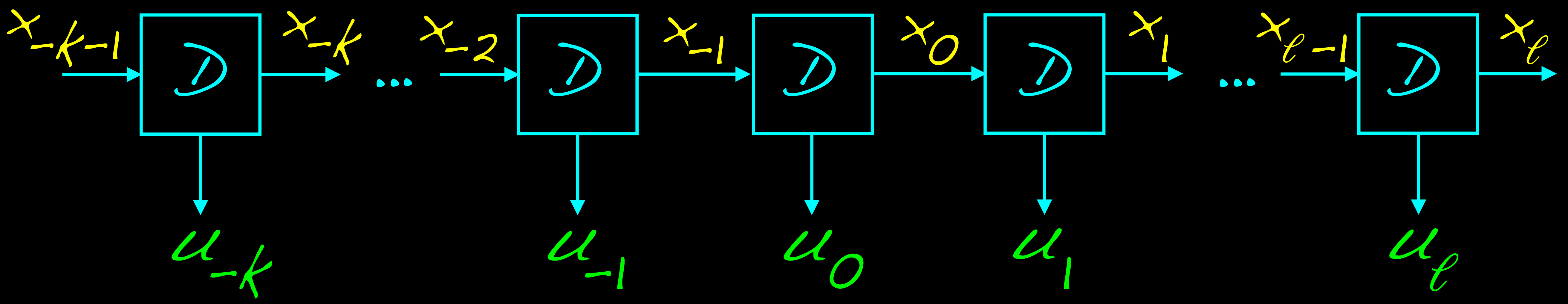


In real life (=in the laboratory):



1-c. General linear structure

The $x_t \in V$ are elements of a (real) vector space, and $\mathcal{D}$ is a collection of linear maps:



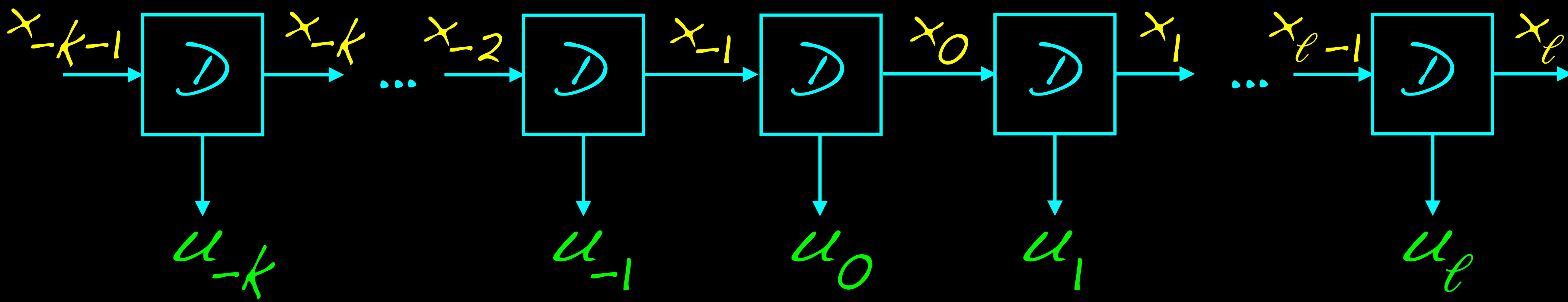
$\mathcal{D}_u : V \to V$ are linear maps, $\tau \in V$, $\pi \in V^*$, s.t.

$\bar{\mathcal{D}} = \sum_u \mathcal{D}_u$ preserves both τ and ω:

$\bar{\mathcal{D}}\tau = \tau$, $\pi \circ \bar{\mathcal{D}} = \pi$, as well as $\pi(\tau) = 1$.

$$P(u_1 u_2 \ldots u_\ell) = \pi \circ \mathcal{D}_{u_1} \circ \mathcal{D}_{u_2} \cdots \circ \mathcal{D}_{u_\ell} \tau$$ (g.u.r.)

I-c. General linear structure



$\mathcal{D}_u : V \to V$ are linear maps, $\tau \in V$, $\omega \in V^*$, s.t.

$\bar{\mathcal{D}} = \sum_u \mathcal{D}_u$ preserves both τ and π, $\pi(\tau)=1$.

$$P(u_1 u_2 \ldots u_\ell) = \pi \circ \mathcal{D}_{u_1} \circ \mathcal{D}_{u_2} \cdots \circ \mathcal{D}_{u_\ell} \tau \qquad \text{(gu.r.)}$$

Unlike classical and quantum case, no a priori guarantee that $P(\underline{u}) \geq 0$. In fact, deciding positivity is undecidable ⚡

[Sontag, J. Comp. Syst. Sci., 1975]

Example. $V = B(\mathbb{C}^2)_{sa} = \mathrm{span}\{\mathbb{1}, X, Y, Z\}$ qubit with $\tau = \mathbb{1}$, $\pi = \frac{1}{2}\mathrm{Tr}$, and the following maps:

$$D_0(A) = \frac{1}{4} |0\rangle\langle 0| A |0\rangle\langle 0|,$$
$$D_1(A) = \frac{1}{4} |1\rangle\langle 1| A |1\rangle\langle 1|,$$
$$D_X(A) = \frac{1}{4} \exp(i\alpha X) A \exp(-i\alpha X),$$
$$D_Z(A) = \frac{1}{4} \exp(i\beta Z) A \exp(-i\beta Z),$$
$$D_T(A) = \frac{1}{4} A^T.$$

When α/π, β/π are irrational, dynamics explores whole Bloch sphere densely. Four-dim. qu.r., but requires 2 qubits for c.p.r.!

* $\underline{u} = u_1 u_2 \ldots u_\ell \longmapsto D_{\underline{u}} = D_{u_1} \circ D_{u_2} \ldots \circ D_{u_\ell}$ is semigroup representation. (Not crucial, just notation.)

* Classical & quantum case: positivity $P(\underline{u}) \geq 0$ enforced by the vector space order...
  Generally: Assume we have convex cones $C \subset V$ and $\tilde{C} \subset C' \subset V^*$, s.t. $\tau \in C$, $\pi \in \tilde{C}$, and the cones are preserved by the transformations, i.e. $D_u C \subset C$, $\tilde{C} D_u \subset \tilde{C}$ for all u.

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Dual cone $C' = \{ f \in V^* : f(x) \geq 0 \ \forall x \in C \}$

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Generally: Assume we have convex cones $C \subset V$ and $\tilde{C} \subset C' \subset V^*$, s.t. $\tau \in C$, $\pi \in \tilde{C}$, and the cones are preserved by the transformations, i.e. $D_u C \subset C$, $\tilde{C} D_u \subset \tilde{C}$ for all u.

Conversely: If $P \geq 0$, then such cones exist, e.g. $C = C_{min} = \overline{\mathrm{cone}\{D_{\underline{u}}\tau : \underline{u} \in \mathbb{M}^*\}}$,

$\tilde{C} = C'_{max} = \overline{\mathrm{cone}\{\pi D_{\underline{u}} : \underline{u} \in \mathbb{M}^*\}}$.

...not unique, could for instance also take dual cone $\tilde{C} = C'$ – call such a C "suitable".

2. Reconstruction of V

* Consider the Hankel-type matrix $\mathcal{H} = (\mathcal{H}_{\underline{u},\underline{v}})$, with $\mathcal{H}_{\underline{u},\underline{v}} = P(\underline{uv}) = P(u_1 u_2 \dots u_\ell v_1 v_2 \dots v_k)$

$$= \mathcal{H}_{\varepsilon,\underline{uv}} = \mathcal{H}_{\underline{uv},\varepsilon}.$$

* If the process P has a quasi-realisation of $\dim V = d$, then

$$\mathcal{H}_{\underline{u},\underline{v}} = (\pi \circ \mathcal{D}_{\underline{u}})(\mathcal{D}_{\underline{v}} \tau),$$

and so $\operatorname{rank} \mathcal{H} \leq d$.

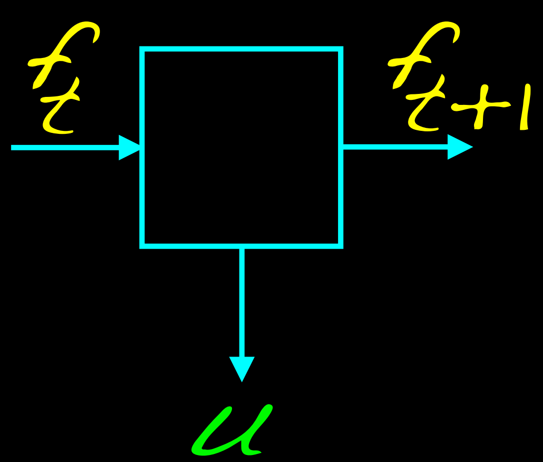
* Consider the Hankel-type matrix $\mathcal{H}=(\mathcal{H}_{\underline{u},\underline{v}})$, with $\mathcal{H}_{\underline{u},\underline{v}} = P(\underline{uv}) = P(u_1 u_2 \dots u_\ell v_1 v_2 \dots v_k)$.

* Conversely, if $\operatorname{rank} \mathcal{H} = r < \infty$: There exists a qu.r. ("regular rep.") with $\dim V = r$, which is the minimum. Any other minimal-dim. qu.r. is similar to the regular one.
[Construction: V = column space of $\mathcal{H}$, and D_u maps $h_{\underline{v}} = \mathcal{H}_{\cdot,\underline{v}}$ to $h_{u\underline{v}} = \mathcal{H}_{\cdot,u\underline{v}}$ - linear because it selects the rows ending in u; $\tau=h_\varepsilon$, $\pi=(1,0,0,\dots)$. Check that it works...]

Interpretation – Finite dimensional regular representation "explains" time series P by the hidden mechanism of generalised probabilistic theory (GPT):

- C and C' are pointed and generating cones;
- $\tau \in int(C)$ and $S := \{f \in C' : f(\tau) = 1\}$ state space;
- $\mathfrak{E} := C \cap (\tau - C)$ "effects" for measurements.

[G. Ludwig & school, 1960s–70s, ...]



$\equiv$ { $f_t \circ D = \Pr\{u|f_t\} f_{t+1}$, relates current & future states, and the output u.

Assume from now on that we "know" $\mathcal{H}$ and the regular representation.

Caveat! In practice, can know only a finite part of $\mathcal{H}$, i.e. some entries or more generally expectation values $\mathrm{Tr}\,\mathcal{H} M_j = \lambda_j$. (*)

Want to find a low-rank completion of $\mathcal{H}$ with (*) and subject to constraints:

(Positivity) $\mathcal{H}_{\underline{u},\underline{v}} \geq 0$,

(Hankel) $\mathcal{H}_{\underline{u},\underline{v}} = \mathcal{H}_{\varepsilon,\underline{uv}} = \mathcal{H}_{\underline{uv},\varepsilon}$,

(Marginals) $\sum_w \mathcal{H}_{\underline{u},\underline{v}w} = \mathcal{H}_{\underline{u},\underline{v}} = \sum_w \mathcal{H}_{w\underline{u},\underline{v}}$

As yet unsolved, but we think that the "usual" tools will do it... [w/ S Flammia & R Küng, w.i.p.]

3. Removing redundancy: quotients

If your model is not minimal, still useful, assuming it has a suitable cone $C \subset V$.

Redundancy: $W = \mathrm{span}\{D_{\underline{u}}\tau : \underline{u} \in \mathbb{M}^*\} \subset V$,

$K = \{\pi D_{\underline{u}} : \underline{u} \in \mathbb{M}^*\}^{\perp} \subset V$.

Null space; $C \cap K = 0$, so we may factor out K...

Reachable space; might as well go to W, with cone $C \cap W$...

3. Removing redundancy: quotients

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$$\mathrm{K} = \{ \pi \mathcal{D}_{\underline{u}} : \underline{u} \in \mathbb{M}^* \}^{\perp} \subset V.$$

$V_0 := \mathcal{W} / \mathrm{K}$,

$C_0 := (C \cap \mathcal{W}) / \mathrm{K} = \{ \omega + \mathrm{K} : \omega \in C \cap \mathcal{W} \}$,

$\tau_0 := \tau + \mathrm{K}$, $\pi_0 := \pi / \mathrm{K}$, $\mathcal{D}^0_u := \mathcal{D}_u / \mathrm{K}$; well-defined because of $\pi(\mathrm{K}) = 0$, $\mathcal{D}_u \mathcal{W} \subset \mathcal{W}$, $\mathcal{D}_u \mathrm{K} \subset \mathrm{K}$.

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$V_0 := W/K$,

$C_0 := (C \cap W)/K = \{w + K : w \in C \cap W\}$,

$\tau_0 := \tau + K$, $\pi_0 := \pi/K$, $D^0_{\underline{u}} := D_{\underline{u}}/K$.

Always a minimal-dim. qu.r., hence is isomorphic to regular, and cone C_0 is suitable.

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$\tau_0 := \tau + K$, $\pi_0 := \pi/K$, $\mathcal{D}^0_u := \mathcal{D}_u/K$.

Classical model, i.e. $V = \mathbb{R}^d$, $C = \mathbb{R}^d_{\geq 0}$, $\tau = (1, \dots, 1)^\top$, π a probability row vector.

C_0 is then a polyhedral cone and every such cone arises in the above way (Fourier-Motzkin elemination). Guaranteed:

$d \leq$ #extremal rays of C, sometimes best.

3'. Quotient of a quantum model

Quantum model, i.e. $V = B(\mathcal{H})_{sa}$, $C = B(\mathcal{H})_{\geq 0}$, $\tau = \mathbb{1}$,
$\pi = \omega$ quantum state, D_u are cp maps.

Once constructed $K \cap W \subset W \subset V$: $C \cap W$ is an operator system, $C_0 = (C \cap W)/K$ a quotient operator system; the D_u^0 preserve C, in fact cp maps in the operator system sense.

[Farenick/Paulsen, Math. Scand. 111:210-243, 2012]

Membership in the cone is an SDP: semi-definite condition of a finite-size matrix with existential real variables.

SDR operator systems:

$\mathbb{1} \in \mathcal{W} = \mathrm{span}\{\mathcal{D}_{\underline{u}}\mathbb{1} \ : \ \underline{u} \in \mathbb{M}^*\} = B(\mathcal{H})_{sa}$,

$K = \{\omega \circ \mathcal{D}_{\underline{u}} : \underline{u} \in \mathbb{M}^*\}^{\perp} \subset B(\mathcal{H})_{sa}$.

Vector space and positive cone:

$V_0 := \mathcal{W}/K$,

$C_0 := (B(\mathcal{H})_{\geq 0} \cap \mathcal{W})/K = \{\omega + K \ : \ \omega \in B(\mathcal{H})_{\geq 0} \cap \mathcal{W}\}$.

Operator system lifts this to $V_0 \otimes B(\mathbb{C}^n)_{sa}$:

$C_n := (B(\mathcal{H} \otimes \mathbb{C}^n)_{\geq 0} \cap \mathcal{W} \otimes B(\mathbb{C}^n)_{sa})/K \otimes \mathbb{1}$

CP maps: $(\mathcal{D}_u \otimes id)C_n \subset C_n$ for all u and n.

[Farenick/Paulsen, Math. Scand. 111:210-243, 2012]

But the $\mathcal{D}_U^o$ remember more than just being cp in the operator system. Indeed,

$$\mathcal{D}_U^o \in \mathscr{P} := \{\Lambda/K : \Lambda \text{ cp on } B(\mathcal{H}),\ \Lambda(\mathcal{W})\subset\mathcal{W},\ \Lambda(K)\subset K\} \subset End(V_0),$$

which is itself an SDR cone. Maybe you don't find it too pretty...it took us a while, too, to see its beauty :-)

$\mathscr{P}=\mathscr{P}(\mathcal{W},K) \subset CP(V_0)$, and in general the inclusion is strict!

[Equality by Arveson's extension theorem for $K=0$ & $\mathcal{W}=B(\mathcal{H})_{sa}$]

4. Reconstructing the vector order?

Task: Find a suitable cone C for the qu.r. $(V, \tau, \pi, \mathcal{D}_u)$, ideally a "nice" one...

Necessarily, $C_{min} \subset C \subset C_{max}$, with (recall)

$$C_{min} = \overline{\mathrm{cone}\{\mathcal{D}_{\underline{u}}\tau : \underline{u} \in \mathbb{M}^*\}},$$

$$C_{max} = \mathrm{cone}\{\pi\mathcal{D}_{\underline{u}} : \underline{u} \in \mathbb{M}^*\}'.$$

Can we choose C polyhedral or SDR?

Difficulty of course that C has to be preserved by the $\mathcal{D}_u$; note that C_{min} & C_{max} satisfy this automatically.

4. Reconstructing the vector order?

Instructive special case: $C = C_{min} = C_{max}$, ruling out a classical model if that is not a polyhedral cone. [Cf. example, where this happens with C=cone over a Bloch sphere.]

Can we construct an example where C is unique and not SDR?! Would provide a process generated by a finite GPT, but w/o quantum realisation...(???)

Related question: Can we find C_{min} & C_{max} that are not even semi-algebraic?

5. Questions, questions, questions

- Low-rank completion of the Hankel matrix?
- Are there GPT models without a finite quantum realisation?
- How to find an SDR cone C of the quotient form W/K such that $D_u \in \mathcal{P}(W,K)$?
- For an SDR operator system V_0, $CP(V_0)$ equals the union of all eligible scarrafoni?
- How to decide complete positivity for SDR operator systems?

QML Startup
(launch date
~1/4/2018)

giuscarrafone.com

Grazie Pino Daniele 💚