Von Neumann's Other Entropy

—observational entropy, coarse-grained states, Petz recovery maps—

ovvero

"The Entropy, The Paradox, and The Observer"

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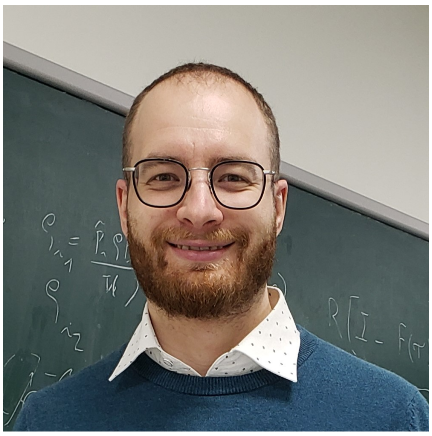


The Observational Entropy Appreciation Club
(www.observationalentropy.com)

Enter the Entropy

von Neumann's entropy

For $\varrho = \sum_{x=1}^{d} \lambda_x |\varphi_x\rangle\langle\varphi_x|$ d-dimensional density matrix ($\lambda_x \geq 0$, $\sum_x \lambda_x = 1$),

$$\boxed{S(\varrho) := -\operatorname{Tr}[\varrho \log \varrho] = -\sum_{x=1}^{d} \lambda_x \log \lambda_x}$$

with the convention $0 \log 0 := 0$.

Unfortunately though:

> *"The expressions for entropy given by the author [previously] are not applicable here in the way they were intended, as they were computed from the perspective of an observer who can carry out all measurements that are possible in principle—i.e., regardless of whether they are* **macroscopic** *[or not]."*
>
> von Neumann, 1929; transl. available in `arXiv:1003.2133`

in formula:

Theorem (least uncertainty)

For ϱ density matrix, $\mathfrak{onb} = \{|\phi_i\rangle\}_i$ orthonormal basis, and $p_i = \langle\phi_i|\varrho|\phi_i\rangle$,

$$S(\varrho) = \min_{\mathfrak{onb}} \left[-\sum_i p_i \log p_i \right] .$$

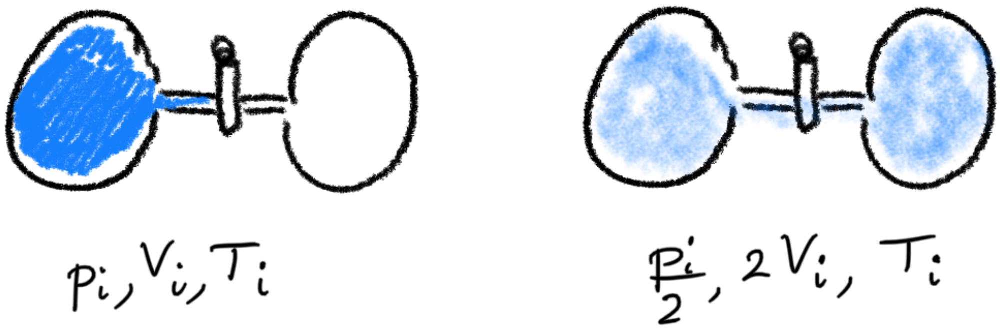
For a more general result, see [M. Dall'Arno and F.B., IEEE TIT, 65(4), 2018].

Enter the Paradox

"Although our entropy expression, as we saw, is completely analogous to the classical entropy, it is still surprising that it is invariant in the normal [Hamiltonian] evolution in time of the system, and only increases with measurements—in the classical theory (where the measurements in general played no role) it increased as a rule even with the ordinary mechanical evolution in time of the system. It is therefore necessary to clear up this apparently paradoxical situation."

von Neumann, book (Math. Found. QM), 1932 (transl. 1955)

free expansion of an ideal gas



$$\boxed{\Delta S(\text{universe}) = nR\ln 2 > 0}$$

invariance of von Neumann entropy

Instead,

Theorem

For any unitary operator U,

$$S(\varrho) = S(U\varrho U^\dagger)\ ,$$

for all density matrices ϱ.

von Neumann's insight (inspired by Szilard's)

"For a classical observer, who knows all coordinates and momenta, the entropy is constant. [...]
The time variations of the entropy are then based on the fact that the observer does not know everything—that he cannot find out (measure) everything which is measurable in principle."

von Neumann, 1932 (transl. 1955)

Enter the Observer

von Neumann's proposal: macroscopic entropy

For

- ϱ density matrix,
- $\mathfrak{P} = \{\Pi_i\}_i$ orthogonal resolution of identity,
- $p_i = \mathrm{Tr}[\varrho\, \Pi_i]$,
- $\Omega_i := \mathrm{Tr}[\Pi_i]$,

$$\boxed{S_{\mathfrak{P}}(\varrho) := -\sum_i p_i \log \frac{p_i}{\Omega_i}}$$

modern generalization: observational entropy

For

- ϱ density matrix,
- **P** $= \{P_i\}_i$ POVM (i.e., $P_i \geq 0$, $\sum_i P_i = \mathbb{1}$),
- $p_i = \mathrm{Tr}[\varrho\, P_i]$,
- $V_i := \mathrm{Tr}[P_i]$,

$$\boxed{S_{\mathbf{P}}(\varrho) := -\sum_i p_i \log \frac{p_i}{V_i}}$$

References:

1. D. Šafránek, J.M. Deutsch, A. Aguirre. *Phys. Rev. A* **99**, 012103 (2019)
2. D. Šafránek, A. Aguirre, J. Schindler, J. M. Deutsch. *Found. Phys.* **51**, 101 (2021)

“observational” = “of the observer”

- von Neumann defines a **macro-observer** as a collection of simultaneously measurable quantities $\{\mathbf{Q}_1, \mathbf{Q}_2, \ldots, \mathbf{Q}_n, \ldots\}$, where $\mathbf{Q}_n = \{Q_{x|n}\}_x$ are POVMs
- $\implies$ there exists one “mother” POVM $\mathbf{P} = \{P_i\}_i$ and a stochastic processing (i.e., cond. prob.) μ such that

$$Q_{x|n} = \sum_i \mu(x|n,i) P_i \ , \quad \forall x, n$$

- $\implies$ “a macro-observer” := “a POVM”—from which all macroscopic measurements (i.e., coarse-grainings) can be simultaneously inferred by stochastic post-processing

Mathematical properties

Umegaki's relative entropy

Definition

For density matrices ϱ, σ,

$$D(\varrho\|\sigma) := \begin{cases} \mathrm{Tr}[\varrho(\log\varrho - \log\sigma)] \ , & \text{if } \operatorname{supp}\varrho \subseteq \operatorname{supp}\sigma \ , \\ +\infty \ , & \text{otherwise} \end{cases}$$

Useful properties:

- $D(A\|B) \geq 0$
- $S(\varrho) = \log d - D(\varrho\|u)$ where $u := d^{-1}\mathbb{1}$
- **monotonicity**: $D(\varrho\|\sigma) \geq D(\mathcal{E}(\varrho)\|\mathcal{E}(\sigma))$ for all channels (i.e., CPTP linear maps) $\mathcal{E}$ and all states ϱ, σ

a bound on the observational entropy

Theorem

For any state ϱ and any POVM $\mathbf{P} = \{P_i\}_i$

$$S(\varrho) \leq S_{\mathbf{P}}(\varrho) \ .$$

Proof.

Given a POVM $\mathbf{P}$, by defining the corresponding CPTP linear map $\mathcal{P}(\bullet) := \sum_i \mathrm{Tr}[P_i \ \bullet] \, |i\rangle\langle i|$, we have ($u = d^{-1}\mathbb{1}$)

$$S_{\mathbf{P}}(\varrho) - S(\varrho) = D(\varrho\|u) - D(\mathcal{P}(\varrho)\|\mathcal{P}(u)) \ ,$$

which is non-negative due to the monotonicity property of the Umegaki quantum relative entropy. □

Petz's theorem

In general, $D(\varrho\|\sigma) \geq D(\mathcal{E}(\varrho)\|\mathcal{E}(\sigma))$.
Question: for which triples $(\varrho, \sigma, \mathcal{E})$ do we have $D(\varrho\|\sigma) = D(\mathcal{E}(\varrho)\|\mathcal{E}(\sigma))$?

Petz (1986,1988)

Answer: if and only if the "transpose channel", i.e.,

$$\widetilde{\mathcal{E}}_\sigma(\bullet) := \sqrt{\sigma}\mathcal{E}^\dagger\left[\frac{1}{\sqrt{\mathcal{E}(\sigma)}}\bullet\frac{1}{\sqrt{\mathcal{E}(\sigma)}}\right]\sqrt{\sigma}$$

satisfies $\widetilde{\mathcal{E}}_\sigma \circ \mathcal{E}(\varrho) = \varrho$. (The other equality $\widetilde{\mathcal{E}}_\sigma \circ \mathcal{E}(\sigma) = \sigma$ is satisfied *by construction*.)

Remark. Notice that $\widetilde{\mathcal{E}}_\sigma$ in general is *not* the linear inverse of $\mathcal{E}$—rather, it is related with the idea of *statistical retrodiction* (more on this later).

consequences for observational entropy

Theorem

$$\boxed{S(\varrho) = S_{\mathbf{P}}(\varrho) \iff \varrho = \sum_i \mathrm{Tr}[\varrho\ P_i]\,\frac{P_i}{V_i}\ .}$$

Proof.

This is a direct consequence of Petz's transpose map theorem:
$S_{\mathbf{P}}(\varrho) - S(\varrho) = D(\varrho\|u) - D(\mathcal{P}(\varrho)\|\mathcal{P}(u)) = 0$ if and only if $\varrho = \widetilde{\mathcal{P}}_u(\mathcal{P}(\varrho))$. By direct inspection, $\widetilde{\mathcal{P}}_u(\mathcal{P}(\varrho)) = \sum_i \mathrm{Tr}[\varrho\ P_i]\, P_i/V_i$. □

Remark. For any POVM **P**, at least one density matrix ϱ exists such that $\widetilde{\mathcal{P}}_u(\mathcal{P}(\varrho)) = \varrho$, e.g., the uniform u.

the resolution of the paradox

- let us start at $t = t_0$ from a state of maximum knowledge, i.e., $S_{\mathbf{P}}(\varrho^{t_0}) = S(\varrho^{t_0})$
- suppose that the system undergoes a unitary evolution, i.e., $\varrho^{t_0} \mapsto \varrho^{t_1} = U\varrho^{t_0}U^\dagger$; then,

$$S_{\mathbf{P}}(\varrho^{t_1}) \equiv -\sum_i \mathrm{Tr}\big[P_i\ (U\varrho^{t_0}U^\dagger)\big] \log \frac{\mathrm{Tr}\big[P_i\ (U\varrho^{t_0}U^\dagger)\big]}{\mathrm{Tr}[P_i]}$$

$$= -\sum_i \mathrm{Tr}\big[(U^\dagger P_i U)\ \varrho^{t_0}\big] \log \frac{\mathrm{Tr}\big[(U^\dagger P_i U)\ \varrho^{t_0}\big]}{\mathrm{Tr}[U^\dagger P_i U]} \equiv S_{U^\dagger \mathbf{P} U}(\varrho^{t_0})$$

- hence, in general, $S_{\mathbf{P}}(\varrho^{t_1}) \equiv S_{U^\dagger \mathbf{P} U}(\varrho^{t_0}) \geq S(\varrho^{t_0}) \equiv S_{\mathbf{P}}(\varrho^{t_0})$, the equality $S_{\mathbf{P}}(\varrho^{t_1}) = S_{\mathbf{P}}(\varrho^{t_0})$ occurring only if $\varrho^{t_0} = \sum_i \mathrm{Tr}[P_i\ \varrho^{t_0}]\, \frac{P_i}{V_i} = \sum_i \mathrm{Tr}\big[(U^\dagger P_i U)\ \varrho^{t_0}\big]\, \frac{U^\dagger P_i U}{V_i}$, that is

$$\boxed{\varrho^{t_0} = \sum_i \mathrm{Tr}\big[P_i\ \varrho^{t_0}\big]\frac{P_i}{V_i} \quad \longmapsto \quad \varrho^{t_1} = \sum_i \mathrm{Tr}\big[P_i\ \varrho^{t_1}\big]\frac{P_i}{V_i}}$$

Generalization to finite differences

a strong bound

What does a finite difference, i.e., $S_{\mathbf{P}}(\varrho) - S(\varrho) > 0$, tell us then?

Theorem

For any density matrix ϱ and any POVM $\mathbf{P} = \{P_i\}_i$,

$$S_{\mathbf{P}}(\varrho) - S(\varrho) \geq D(\varrho \| \varrho_{\rm cg}) ,$$

where $\varrho_{\rm cg} := \widetilde{\mathcal{P}}_u(\mathcal{P}(\varrho)) = \sum_i \mathrm{Tr}[\varrho\ P_i] \dfrac{P_i}{V_i}$ is the coarse-grained state inferred from the measurement's data.

Remark. Notice how $\varrho_{\rm cg}$ only depends on data available to the observer: the outcome probabilities p_i and the POVM elements P_i.

triangle *equality* for observational entropy

Theorem

Given a d-dimensional system, a density matrix $\varrho = \sum_{x=1}^d \lambda_x |\varphi_x\rangle\langle\varphi_x|$, and a POVM $\mathbf{P} = \{P_i\}_i$, let us define two joint probability distributions:

$$P_F(x,i) := \lambda_x \, \mathrm{Tr}[|\varphi_x\rangle\langle\varphi_x|\ P_i] , \qquad P_R(x,i) := p_i \, \mathrm{Tr}\left[|\varphi_x\rangle\langle\varphi_x|\ \frac{P_i}{V_i}\right] .$$

Then,

$$S_{\mathbf{P}}(\varrho) - S(\varrho) = D(P_F \| P_R) .$$

interpretation: prediction and retrodiction

- start from $P_F(x,i) = \lambda_x \langle \varphi_x | P_i | \varphi_x \rangle =: \lambda_x \pi_F(i|x)$
- notice that $\sum_i P_F(x,i) = \lambda_x$ and $\sum_x P_F(x,i) = \mathrm{Tr}[\varrho\ P_i] = p_i$
- write this as $\boldsymbol{\lambda} \xrightarrow{\boldsymbol{\pi}} \boldsymbol{\pi}[\boldsymbol{\lambda}] \equiv \boldsymbol{p}$
- take now $P_R(x,i) = p_i \langle \varphi_x | \frac{P_i}{V_i} | \varphi_x \rangle =: p_i \pi_R(x|i)$
- notice that $\pi_R(x|i) = \frac{\langle \varphi_x | P_i | \varphi_x \rangle}{\sum_x \langle \varphi_x | P_i | \varphi_x \rangle} = \frac{d^{-1} \langle \varphi_x | P_i | \varphi_x \rangle}{\sum_x d^{-1} \langle \varphi_x | P_i | \varphi_x \rangle} = \frac{u_x \pi_F(i|x)}{\sum_x u_x \pi_F(i|x)}$
- hence $\pi_R(x|i)$ is the Bayesian inverse $\widetilde{\boldsymbol{\pi}}_{\boldsymbol{u}}$ of the process $\boldsymbol{u} \xrightarrow{\boldsymbol{\pi}} \boldsymbol{\pi}[\boldsymbol{u}]$

in the language of Jeffrey's probability kinematics

- P_F corresponds to the prediction $\boldsymbol{\lambda} \xrightarrow{\boldsymbol{\pi}} \bullet$: the inference about i
- P_R corresponds to the retrodiction $\bullet \xleftarrow{\widetilde{\boldsymbol{\pi}}_{\boldsymbol{u}}} \boldsymbol{p}$: the inference about x that a **completely uninformed Bayesian agent** would do, if given information about i in the form of the probability distribution $\boldsymbol{p}$.

The equality $S_{\mathbf{P}}(\varrho) = S(\varrho)$ occurs **if and only if** predictor and retrodictor agree.

Watanabe's contention

"The phenomenological oneway-ness of temporal developments in physics is due to **irretrodictability**, *and not due to irreversibility."*

Satosi Watanabe (1965)

The Second Law of Thermodynamics is not about the "arrow of time", but about the **arrow of inference**.

- F.B. and V. Scarani, *Fluctuation relations from Bayesian retrodiction*, PRE (2021)
- C.C. Aw, F.B., and V. Scarani, *Fluctuation theorems with retrodiction rather than reverse processes*, AVS Quantum Science (2021)

Conclusions

take-home messages

When the use of von Neumann entropy in thermodynamics is problematic, try consider observational entropy (OE) instead, because:

1. **von Neumann told you so!** OE has a fully operational/inferential definition
2. OE unifies Gibbs and Boltzmann entropies
3. OE solves interpretational paradoxes
4. OE fits nicely within recent developments in quantum mathematical statistics (e.g., approximate Petz recovery)
5. OE has built-in a concept of Bayesian prediction and retrodiction

THE END: THANK YOU!