Retrodiction in Stochastic Thermodynamics

Francesco Buscemi* (joint work with Valerio Scarani)

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*www.quantumquia.com

New physics!!

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Initial data from the Muon g-2 experiment have excited particle physicists searching for undiscovered subatomic particles and forces

By Daniel Garisto on April 7, 2021 أعرض هذا باللغة العربية

Muon g-2 magnetic storage ring, seen here at Brookhaven National Laboratory in New York State before its 2013 relocation to Fermi National Accelerator Laboratory in Illinois. Credit: Alamy

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New "physics"??


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A step towards LIMITLESS energy: Loophole found in a fundamental law of physics may lead to infinite power

- The finding may mean it's possible to create perpetual motion machines
- These machines can spin for eternity without losing any energy
- The four laws of thermodynamics set the physical rules for our universe
- Researchers found a way to bypass the second law of the four
- They have since projected a quantum system in which energy can be recycled

By HARRY PETTIT FOR MAILONLINE
PUBLISHED: 14:00 BST, 3 November 2016 | UPDATED: 17:03 BST, 3 November 2016

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Einstein once boldly claimed that the Laws of Thermodynamics were the only physical theory of the universe that will 'never be overthrown'.

That all changed late last month, when scientists from the Argonne National Laboratory at the University of Chicago found a loophole in the system - one that allows them to break the second law of thermodynamics.

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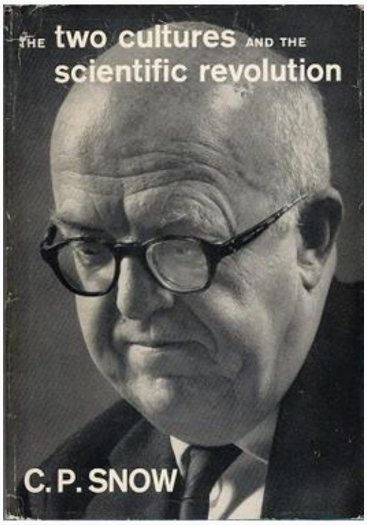
The Second Law is special

"The law that entropy always increases holds, I think, the supreme position among the laws of Nature. [...] If your theory is found to be against the Second Law of Thermodynamics I can give you no hope; there is nothing for it to collapse in deepest humiliation."

A.S. Eddington

"[...] the only physical theory of universal content concerning which I am convinced that, within the framework of the applicability of its basic concepts, it will never be overthrown." A. Einstein

Have you read a work of Shakespeare's?



"Once or twice I have been provoked and have asked the company how many of them could describe the Second Law of Thermodynamics. The response was cold: it was also negative. Yet I was asking something which is about the equivalent of: Have you read a work of Shakespeare's?" C.P. Snow

The "to be or not to be" of thermodynamics

Clausius Inequality

$$\langle \Delta S_{\text{tot}} \rangle \geq 0$$

Why should the above inequality be so "special"? What does it *really* say?

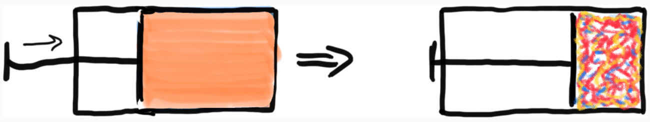
That is the question.

That is the question!

" No one understands entropy very well."

von Neumann (apocryphal)

The Second Law "without entropy"

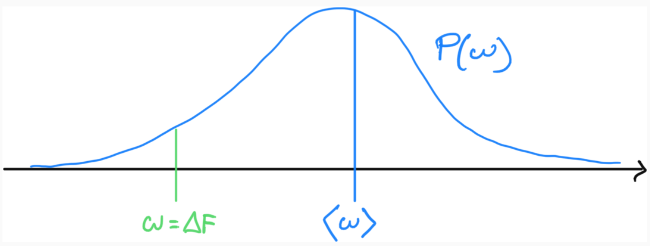


Clausius' inequality (1865):

$$\langle W \rangle \geq \Delta F$$

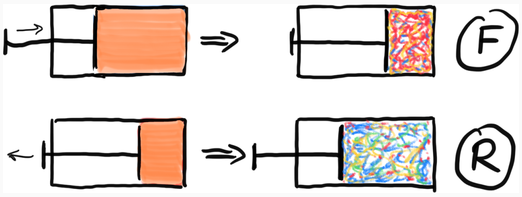
Jarzynski's equality (1997):

$$\left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F}$$



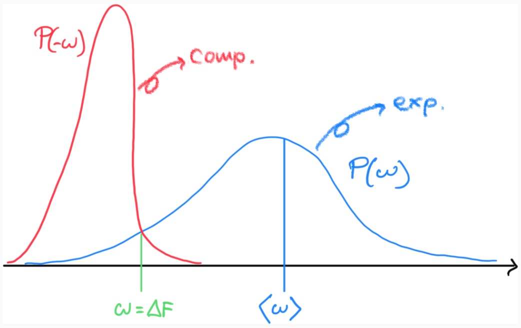
Jarzynski $\Longrightarrow$ Clausius

The Second Law and irreversibility



Crooks' fluctation theorem (1999)

$$\frac{P_F(W)}{P_R(-W)} = e^{\beta(W-\Delta F)}$$



Crooks $\implies$ Jarzynski $\implies$ Clausius

Usual explanation

Crooks' theorem, and hence Jarzynski's relation, and hence the Second Law, all rely on two assumptions satisfied at equilibrium:

1. thermal equilibrium: initial distribution is $P(\xi) \propto e^{-\beta\epsilon(\xi)}$
2. microscopic reversibility: molecular processes and their reverses occur at the same rate

But, again: why does the Second Law feel so "special" then?

Is that because of some kind of "special" microscopic balancing mechanism?

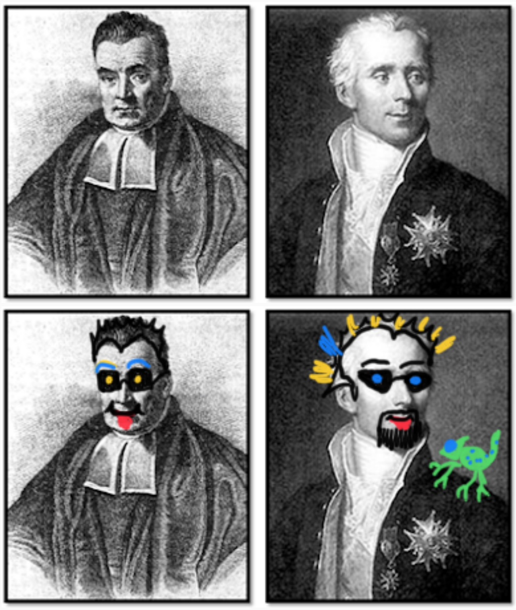
A hint from Ed Jaynes

"To understand and like thermo we need to see it, not as an example of the n-body equations of motion, but as an example of the logic of ***scientific inference****."*

E.T. Jaynes (1984)

First idea: reverse process as Bayesian retrodiction

The Bayes-Laplace Rule



Inverse Probability Formula

$$\underbrace{\mathcal{P}(H|D)}_{\text{inv. prob.}} \propto \underbrace{\mathcal{P}(D|H)}_{\text{likelihood}} \underbrace{\mathcal{P}(H)}_{\text{prior}}$$

where H is a hypothesis, D is the result of observation (i.e., evidence)

postmodern Bayesianism!

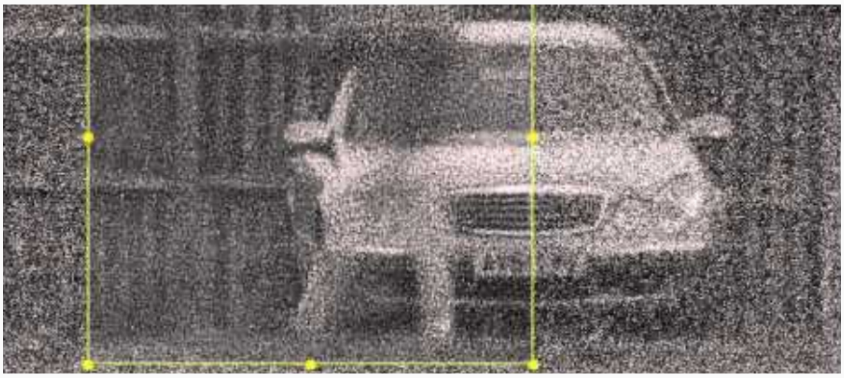
Meanings of the inverse probability

- it is the main *tool* of Bayesian statistics for problems like:
  - estimation (e.g.: how many red balls are in an urn?)
  - decision (e.g.: is ACME's stock a good investment? should I buy some?)
  - predictive inference (e.g.: weather forecasts)
  - retrodictive inference (e.g.: what kind of stellar event possibly caused the Crab Nebula?)
- it measures the degree of belief that a rational agent should have in one hypothesis, among other mutually exclusive ones, given the data

Noisy data and uncertain evidence

BUT! Bayes-Laplace Rule *does not* tell us how to update the prior in the face of uncertain data...

- suppose that a noisy observation suggests a probability distribution $\mathcal{Q}(D)$ for the data (e.g., the license plate no.)



- how should we update our prior $\mathcal{P}(H)$ given *uncertain evidence* in the from $\mathcal{Q}(D)$?

Jeffrey's rule of probability kinematics

Vanilla Bayes:

$$\mathcal{P}(H|D) = \mathcal{P}(D|H)\mathcal{P}(H)/\mathcal{P}(D)$$

Extended Bayes:

$$\mathcal{P}(H|\mathcal{Q}(D)) = ?$$

Jeffrey's conditioning* (1965)

$$\mathcal{P}(H|\mathcal{Q}(D)) = \sum_D \underbrace{\mathcal{P}(H|D)}_{\text{inv. prob.}} \mathcal{Q}(D)$$

$$= \sum_D \frac{\mathcal{P}(D|H)\mathcal{P}(H)}{\sum_H \mathcal{P}(D|H)\mathcal{P}(H)} \mathcal{Q}(D)$$

* Jeffrey's rule was introduced *ad hoc*, but it can be proved from Bayes-Laplace Rule and Pearl's method of virtual evidence (1988)

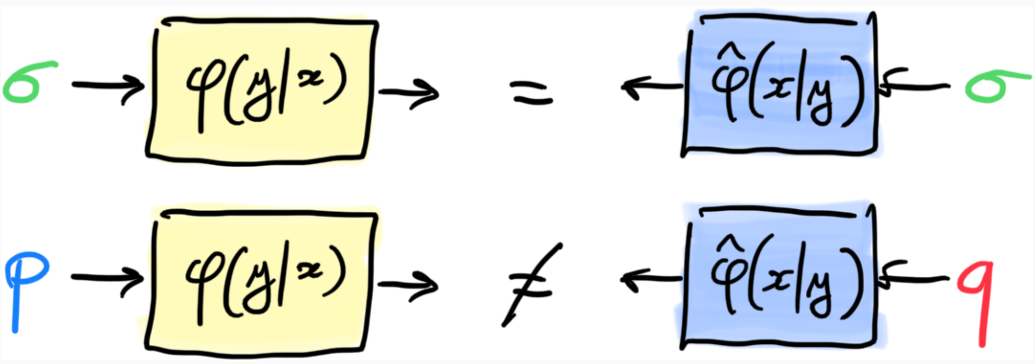
Construction of the reverse process

- **physical setup**:
  - a stochastic transition rule: $\varphi(y|x)$
  - a steady (viz. invariant) state: $\sum_x \varphi(y|x)\sigma(x) = \sigma(y)$
- **Bayesian inversion at the steady state**:

$$\sigma(y)\hat{\varphi}(x|y) := \sigma(x)\varphi(y|x) \quad \iff \quad \frac{\varphi(y|x)}{\hat{\varphi}(x|y)} = \frac{\sigma(y)}{\sigma(x)}$$

- **two priors**:
  - predictor's prior: $p(x)$
  - retrodictor's prior $q(y)$
- **two processes**:
  - forward process (prediction): $\mathcal{P}_F(x,y) = \varphi(y|x)p(x)$
  - reverse process (retrodiction): $\mathcal{P}_R(x,y) = \hat{\varphi}(x|y)q(y)$

A picture



- at the steady state: prediction = retrodiction
- otherwise: asymmetry (irreversibility, *irretrodictability*)

Measures of statistical divergence

Second idea: fluctuation relations as measures of *statistical divergence* between $\mathcal{P}_F(x,y)$ and $\mathcal{P}_R(x,y)$

- relative entropy:

$$D(\mathcal{P}_F \| \mathcal{P}_R) := \left\langle -\ln \frac{\mathcal{P}_R(x,y)}{\mathcal{P}_F(x,y)} \right\rangle_F =: \langle -\ln r(x,y) \rangle_F$$

$\rightsquigarrow$ more generally, one can use $D_f(\mathcal{P}_R \| \mathcal{P}_F) := \langle f(r(x,y)) \rangle_F$

- introduce probability density functions

$\rightsquigarrow$ $\Omega(x,y) := f(r(x,y))$

$\rightsquigarrow$ $\mu_F(\omega) := \sum_{x,y} \delta[\omega - \Omega(x,y)]\ \mathcal{P}_F(x,y)$

$\rightsquigarrow$ $\mu_R(\omega) := \sum_{x,y} \delta[\omega - \Omega(x,y)]\ \mathcal{P}_R(x,y)$

$$\Longrightarrow \quad \langle \omega \rangle_F = D_f(\mathcal{P}_R \| \mathcal{P}_F)$$

From f-divergences to f-fluctuation theorems

- for $f : \mathbb{R}^+ \to \mathbb{R}$ invertible

f-Fluctuation Theorem

$$\mu_R(\omega) = f^{-1}(\omega)\mu_F(\omega) \quad \Longrightarrow \quad \langle f^{-1}(\omega) \rangle_F = 1$$

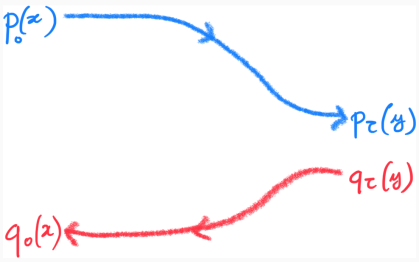
$\rightsquigarrow$ for $f(u) = -\ln u$, we have $f^{-1}(v) = e^{-v}$, that is

$$\frac{\mu_F(\omega)}{\mu_R(\omega)} = e^{\omega} \quad \Longrightarrow \quad \left\langle e^{-\omega} \right\rangle_F = 1$$

further discussions in `arXiv:2009.02849`

Examples

Example: driven Hamiltonian evolution



- driving protocol: $H(0) \to H(t) \to H(\tau)$
- $H(0) = \sum_x \epsilon_x \pi_x$, $H(\tau) = \sum_y \eta_y \pi'_y$
- $\varphi(y|x) = \delta_{y,y(x)}$, i.e., one-to-one
- $\sigma(x) = d^{-1} \implies \varphi(y|x) = \hat{\varphi}(x|y)$
- $p_0(x) = e^{\beta(F-\epsilon_x)}$, $q_\tau(y) = e^{\beta(F'-\eta_y)}$

In this case, for the choice $f(u) = -\ln u$,

$$\Omega(x,y) = \ln \frac{\mathcal{P}_F(x,y)}{\mathcal{P}_R(x,y)} = \ln \frac{\sigma(y)p(x)}{\sigma(x)q(y)} = \ln \frac{p(x)}{q(y)}$$
$$= \beta(F - \epsilon_x + F' + \eta_y) = \beta(W - \Delta F)$$

$$\implies \frac{\mu_F(W)}{\mu_R(W)} = e^{\beta(W-\Delta F)}$$

Example: nonequilibrium steady states

- stochastic process $\varphi(y|x)$ with non-thermal steady state $\sigma(x)$
- thermal equilibrium priors: $p(x) = q(x) \propto e^{-\beta\epsilon_x}$
- fluctuation variable (total stochastic entropy production):
  $\omega = \ln \frac{\mathcal{P}_F(x,y)}{\mathcal{P}_R(x,y)} = \ln \frac{p(x)}{q(y)} \frac{\sigma(y)}{\sigma(x)} = \beta(\epsilon_y - \epsilon_x) + (\ln\sigma(y) - \ln\sigma(x))$
- *nonequilibrium potential*: $V(x) := -\frac{1}{\beta}\ln\sigma(x)$ (e.g., Manzano&al 2015)
- $\left\langle e^{\beta(\Delta E - \Delta V)}\right\rangle_F = 1$, but $\left\langle e^{\beta\Delta E}\right\rangle_F =$ "efficacy"
- $\implies$ nonequilibrium potentials (usually introduced *ad hoc*) are understood here as remnants of Bayesian inversion

But why known relations are compatible with Bayesian inversion?

Is that a necessity?

Sketch argument

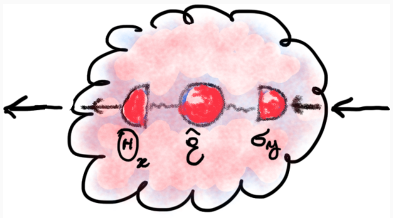
- $D(\mathcal{P}_F \| \mathcal{P}_R) = \left\langle \ln \frac{\mathcal{P}_F(x,y)}{\mathcal{P}_R(x,y)} \right\rangle_F$
- let us impose that the fluctuation variable is a **microstate function**: $\ln \frac{\mathcal{P}_F(x,y)}{\mathcal{P}_R(x,y)} = \Omega(x,y) \overset{!}{=} F'(y) - F(x)$
  - $\implies \frac{\mathcal{P}_F(y|x)}{\mathcal{P}_R(x|y)} = \frac{G'(y)}{G(x)}$
  - $\implies G(x)\mathcal{P}_F(y|x) = G'(y)\mathcal{P}_R(x|y)$
  - sum over $x \implies G'(y) = \sum_x G(x)\mathcal{P}_F(y|x)$
- $\implies \mathcal{P}_R(x|y) = \frac{1}{\sum_x G(x)\mathcal{P}_F(y|x)} G(x)\mathcal{P}_F(y|x)$

Hence, a Bayesian inverse-like form for the reverse process is **inevitable** if we want the (total stochastic) entropy production to be a **microstate function**!

What about the quantum case?

Quantum retrodiction and the Petz map

- assume $\varphi(y|x) = \mathrm{Tr}[\Pi_y\ \mathcal{E}(\rho_x)]$
- let $\sigma(x)$ be invariant distribution
- according to the formalism of *quantum retrodiction*:
  - $\Sigma := \sum_x \sigma(x)\rho_x$
  - $\hat{\rho}_y := \frac{1}{\sigma(y)}\sqrt{\mathcal{E}(\Sigma)}\Pi_y\sqrt{\mathcal{E}(\Sigma)}$
  - $\hat{\Pi}_x := \sigma(x)\frac{1}{\sqrt{\Sigma}}\rho_x\frac{1}{\sqrt{\Sigma}}$
  - $\hat{\mathcal{E}}(\cdot) := \sqrt{\Sigma}\left\{\mathcal{E}^\dagger\left[\frac{1}{\sqrt{\mathcal{E}(\Sigma)}}(\cdot)\frac{1}{\sqrt{\mathcal{E}(\Sigma)}}\right]\right\}\sqrt{\Sigma}$
- Bayesian inversion works seamlessly
  $\hat{\varphi}(x|y) = \mathrm{Tr}[\hat{\Pi}_x\ \hat{\mathcal{E}}(\hat{\rho}_y)]$



Some remarks

- the Petz recovery map is a form of quantum Bayes–Laplace rule
- to a unique Bayes–Laplace rule there correspond infinite possible "rotated" Petz maps
- retrodiction (both classical and quantum) depends on the choice of reference prior
- exceptions are unitary channels, for which:
  1. there is a unique Petz reverse (the retrodiction is independent of the choice of prior, and all rotated Petz maps coincide)
  2. retrodiction and (linear) inversion coincide

Conclusions

Three messages:

- the Second Law is special among the laws of physics, because it is in fact a law of logic
- retrodiction as the logical foundations of fluctuation theorems
- quantum retrodiction also follows seamlessly using Petz recovery map

thank you