Review

#23 PHYSICS OF INFORMATION

1

Thermodynamics → Dynamics of heat

states | Dynamics

Equilibrium Thermodynamics

Statistical Mechanics

Statistical dynamics

stochastic Thermodynamics

$$S(cE, cV, cN) = c\,S(E,V,N)$$

$$P(x) = \frac{e^{-\beta E(x)}}{Z}$$

Models of dynamics

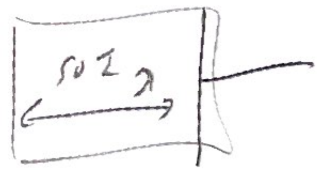
$$\frac{P_F(x)}{P_R(\tilde{x})} = e^{+\Delta S}$$

$$\boxed{\frac{\partial \hat{p}}{\partial t} = \Omega p}$$

Statistical Mechanics

Constant temperature bath

β



Gibbs/Canonical Ensemble
"Boltzmann Distribution"

inverse temperature $= \frac{1}{k_B T}$

$$\boxed{P(x|\lambda) = \frac{e^{-\beta E(x|\lambda)}}{Z}}$$

Internal energy

← partition function

⇐ Do Not Forget

Thermodynamic Equilibrium

Idealized boundary.

Canonical Ensemble.

$$Z = e^{-\beta F}$$ ← free energy

$$\frac{\partial \beta F}{\partial \beta} = -\frac{\partial \ln Z}{\partial \beta} = \langle E \rangle$$

$$\beta F \overset{eq}{=} -\ln Z = \beta \langle E \rangle - S$$

Thermodynamic Equilibrium

Entropy

$$S = - \sum P(x) \ln P(x)$$

k_B belongs in front of the temperature, or better $k_B = 1$

Entropy is maximized at Thermodynamic Equilibrium

T $\langle \Delta S \rangle \geq 0$ Entropy increases in direction of time called the future.
(careful with definitions)

Equilibrium – There is no arrow of time. Past & future look statistically identical

Macroscopic Thermodynamics $\quad cS(E,V,N) \overset{TL}{\simeq} S(cE, cV, cN)$

1st order homogenius function $\quad$ see Callen 1991

$$S = \beta E + -\beta_p V + \beta \mu N$$

pressure $\quad$ chemical potential

$$\frac{1}{K_B T} = \beta = \left.\frac{\partial S}{\partial E}\right|_{V,N}$$

|| Inverse temp is change in entropy with change in energy.

(other relations, e.g. Kinetic temperature, ideal gas law are consequences)

Kinetic energy

$$\langle K \rangle = \frac{3}{2} K_B T N$$

Free Energy

$$\beta F = -\ln Z \quad \text{(equilibrium)}$$

$$= -S + \beta \langle E \rangle \quad \leftarrow \text{valid out-of equilibrium}$$

$$\beta \Delta F \leq \beta \langle W \rangle = \beta W^{rev}$$

$\uparrow$ in or out of equilibrium

$$\beta \Delta F = D(P^{neq} \| P^{eq}) = \sum P(x) \ln \frac{P(x)}{e^{-\beta E(x)}/Z}$$

Work & Heat

$$\frac{dE(x,\lambda)}{dt} = \underbrace{\frac{\partial E}{\partial x}\frac{dx}{dt}\,dt}_{\text{Heat}} + \underbrace{\frac{\partial E}{\partial \lambda}\frac{\partial \lambda}{\partial t}\,dt}_{\text{"Thermodynamic" work}}$$

(not as simple as force × displacement)

Markov
(Back at 6) Detailed Balance (Microscopic Reversibility)

$\frac{P(x|\lambda_t)}{P(\tilde{x}|\tilde{\lambda}_t)} = e^{+\beta Q}$ ~~$t = e^{-\beta \Delta E}$~~

~~$\pi(x)$ $P(x\to$~~

$\pi(x)\, P(x \to x') = \pi(x')\, P(x' \to x)$

Time Reversal Symmetric

7

Markov!

weak coupling to environment

Cellular Automata

Statistical Dynamics

deterministic / stochastic
open / closed
classical / Quantum
discrete time / continuous time
discrete state / continuous states

Liouvillian

$\frac{\partial \rho}{\partial t} = \mathcal{L}\rho$

Markov Chain

DTMC
$p' = M p$

CTMC
$\frac{\partial p}{\partial t} = Q p$

open Quantum

CPTP maps
Quantum Operation $\rho' = S\rho$

Lindblad dynamics
Quantum Master Eq. $\frac{\partial \rho}{\partial t} = -i\mathcal{L}\rho$

closed

classical mechanics
$m\ddot{x} = f$

Quantum mechanics
∂

open

Langevin dynamics
$m\ddot{x} = f - \gamma\dot{x} + \sqrt{\frac{2\gamma}{\beta}}\,\xi$

Brownian dynamics
$\dot{x} = \frac{1}{\gamma} f(x) + \sqrt{\frac{2}{\beta\gamma}}\,\xi(t)$

Simple Model: Foundations of stat. mech.
use the simplest dynamics that captures the physics of interest

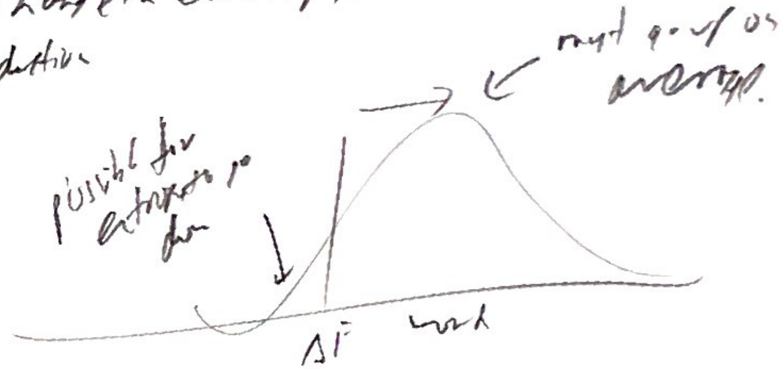
Fluctuation Theorems

Dynamics Time Reversal Symmetric

→ what breaks t.r.s is change in entropy.

$$\frac{P(x \mid \Lambda)}{P(\tilde{x} \mid \tilde{\Lambda})} = e^{+\Delta S} \leftarrow \text{entropy production}$$

$$= e^{-\beta Q}$$



$$= \text{FT} \quad \frac{P_F(W)}{P_R(-W)} = e^{+\beta W \mp \beta \Delta F}$$

Jarzynski

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

Jensen inequality

$$\beta F \leq \beta \langle W \rangle$$

Clausius $\langle \Delta S^{tot} \rangle \geq 0$

$A = -\frac{\partial \Delta F}{\partial \lambda}$ generalized force

Linear Response

$$\langle \delta B(t_0) \rangle_{t_0} \overset{MLR}{=} \frac{\partial \lambda}{\partial t}\Big|_{t_0} \underbrace{\int_0^\infty \langle \delta A(t)\ \delta B(0) \rangle^{eq}_{\lambda_0}}_{\text{eq time correlation function}} = -\frac{\partial \lambda}{\partial t}\Big|_0 \gamma$$

friction coefficient

Microscopic friction $\Rightarrow$ fluctuations, long correlations, long relaxation time

$\rightarrow$ large friction

Entropy

Thermodynamics & The Physics of Information

Entropy $S = -\sum P(x) \log P(x)$

units

base	2	e	10
units	bits	nats	digits

$2^{10} \approx e^{7} \approx 10^{3}$

$1024 \approx 1096.6\ldots \approx 1000$

10 bits $\approx$ 7 nats $\approx$ 3 digits

Joint $S(A,B)$

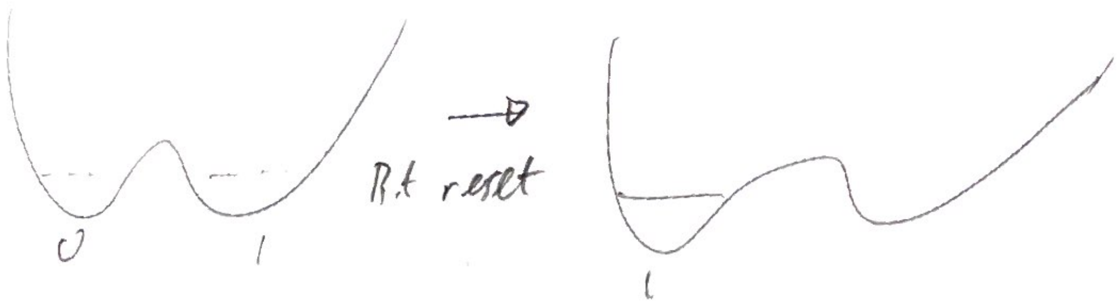
Conditional $S(A|B)$

Mutual Information $I(A:B) = \sum P(x,y) \ln \frac{P(x,y)}{P(x)P(y)}$ ⟸ Information is correlations

Relative $D(A\|B) = \sum P_A(x) \ln \frac{P_A(x)}{P_B(x)}$ (generalizes entropy for continuous systems)

Information is Physical

Thermodynamics = dynamics of heat



Thermodynamic cost of $\frac{1}{\beta} \ln 2$ work

Landauer's principle

Family trees

Kirkwood

DAVID CHANDLER

Chris Jarzynski

~25

Bernard Smit

Greg Voth
Ka Lum
Gavin Crooks
Phill Geissler
David Limmer
Peter Bolhuis
Christoph Dellago
Kranthi Mandadapu

David Sivak
Grant Rotskoff
Steve Whitelam
Todd Gingrich
Asaph Widmer-Cooper
Suri Vaikuntanathan
Jordan Horowitz
Sebastian Deffner

Katie Klymko