

# Information Theory and Networks

## Lecture 32: Information Theory, the Universe and Everything

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October 31, 2013

# Part I

## Information Theory, the Universe, and Everything

Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, except for one or two small points. The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you any more.

*Arnold Sommerfeld*

Nothing in life is certain except death, taxes and the second law of thermodynamics. All three are processes in which useful or accessible forms of some quantity, such as energy or money, are transformed into useless, inaccessible forms of the same quantity. That is not to say that these three processes don't have fringe benefits: taxes pay for roads and schools; the second law of thermodynamics drives cars, computers and metabolism; and death, at the very least, opens up tenured faculty positions.

*Seth Lloyd, writing in Nature 430, 971 (26 August 2004); doi:10.1038/430971a*

# Section 1

## Basic Physics

# Some basic gas physics

- Ideal (classical) gas:
  - ▶ atoms/molecules are indistinguishable, hard spheres
  - ▶ there are a lot of them:
    - ★ Avogadro's constant  $\simeq 6.0 \times 10^{23}/mole$
    - ★ is the number of constituent particles in one mole of a given substance
  - ▶ they bounce elastically off barriers or each other
    - ★ energy is conserved
    - ★ Newton's laws observed (momentum conserved)
  - ▶ no other significant forces on them
    - ★ no friction
    - ★ ignore gravity
    - ★ no other interactions (e.g., no attraction or repulsion)
    - ★ ignore relativity and quantum mechanics
  - ▶ average distance is much larger than size of particles
    - ★ time of collisions is much smaller than time between collisions
- Reasonable approximation for many gases
  - ▶ at typical earth pressures and temperatures

# Macro- vs Micro-state

- Micro-state is everything about all  $n$  particles

- ▶ location of all particles (in 3 space)
- ▶ velocity of all particles (in 3 space)

so there are  $6n$  co-ordinates

- Macro-state

- ▶ We can't keep track of all that, and don't really need it anyway
- ▶ So let's only look at macroscopic properties of the gas
- ▶ e.g.,
  - ★ temperature,  $T$  (in Kelvin)
  - ★ pressure,  $P$  (in Pascals = Newtons per  $m^2$ )
  - ★ volume,  $V$  (in SI units, e.g.,  $m^3$ )
  - ★ number of particles,  $N$  (in moles)
- ▶ state equation for ideal gas

$$PV = NRT$$

where  $R = 8.314 JK^{-1} mol^{-1}$  is the gas constant.

# Macro-state

$$PV = NRT$$

- temperature,  $T$  (in Kelvin)
  - ▶ proportional to the average kinetic energy of particles
  - ▶ kinetic energy of a particle is  $E_p = \frac{1}{2}mv^2$
- pressure,  $P$  (in Pascals = Newtons per  $m^2$ )
  - ▶ created by particles bouncing against the boundary
  - ▶ obviously also related to velocity
    - ★ force  $F = ma$
  - ▶ also related to the density of impacts, which depends on
    - ★ volume
    - ★ number of particles
    - ★ velocity

Note that there are LOTS of microstates (or configurations) that correspond to any given set of macroscopic properties.

# Extensive vs Intensive properties

## Definition (Extensive)

We say a macroscopic property of matter is **extensive** if it is proportional to the **size** of the system (i.e.,  $N$ ).

e.g., total energy, mass, volume, ...

## Definition (Intensive)

We say a macroscopic property of matter is **intensive** if it does not depend on the **size** of the system.

e.g., temperature, density, pressure, ...



# Equilibrium

- Often we consider systems in **dynamic equilibrium**
  - ▶ macroscopic properties aren't changing in time
    - ★ macroscopic variables are therefore adequate descriptors
    - ★ two systems in equilibrium aren't exchanging macroscopic fluxes
    - ★ assumption that macroscopic properties are approximately uniform
  - ▶ not traditional static equilibrium
    - ★ where forces are balanced so system is static
    - ★ dynamic equilibrium allows particles to move (complexly)
- Any transient phenomena have had time to die down
  - ▶ they should die down quickly for large random systems, like a typical gas, but obviously don't change so quickly in other systems, e.g., heating one end of a non-conductive object.
- Specifics depend on the nature of the system, but in general there is an implication that we are in low energy state, or local minimum
- “0th” law of thermodynamics: “if two systems are both in thermal equilibrium with a third system then they are in thermal equilibrium with each other”

# Thermodynamics

- What happens when we change something?
  - ▶ e.g., take a balloon and heat it?
    - ★ pressure and  $N$  approximately constant
    - ★ volume must increase in proportion to temperature
  - ▶ e.g., allow a gas to expand into a larger area
    - ★  $N$  constant
    - ★ pressure and/or temperature will decrease
  - ▶ e.g., put balloon in denser gas (at same temperature)
    - ★  $N$  and temperature constant
    - ★ volume of balloon changes in response to pressure change
- When we change something we do **work**, or the system does **work** on its surroundings
  - ▶ to understand work, we need to understand heat and energy a little better

# Heat

- Remember that temperature is proportional to the average kinetic energy of our gas particles
- Heat is a measure of total kinetic energy
  - ▶ **heat capacity** is the amount of heat energy required to change the temperature of an object/gas by a given amount
    - ★ units = joules per Kelvin
    - ★ for a gas, measure it at constant volume
    - ★ **specific heat capacity** is the heat capacity per mole

$$C = \frac{\Delta Q}{\Delta T}$$

where

- ★  $C$  is heat capacity
- ★  $\Delta Q$  is transfer of heat
- ★  $\Delta T$  is change in temperature

# Internal Energy

- **Internal Energy**  $U$  is the energy to “create” the system
  - ▶ create doesn't mean *ab initio*
  - ▶ means get the system to the state its in
  - ▶ only model particles of interest (not e.g. the walls)
- Consists of
  - ▶ kinetic energy
  - ▶ potential energy
    - ★ resulting from interactions between particles or an external force
- For the ideal gas, we'll assume potential is negligible

$$U = CNT$$

- Changes

$$\Delta U = \Delta Q + \Delta W$$

- ▶  $\Delta Q$  is **heat** added (or lost)
- ▶  $\Delta W$  is work done on the system
  - ★ e.g., by changing the pressure
  - ★ e.g., by changing the volume
- ▶ This is the **1st law of thermodynamics**

# Work

- 1st Law gives an implicit definition of **work**
  - ▶ implicitly it is measured in units of energy (Joules)
- We can do better
  - ▶ origin of idea of work is earlier, e.g., work of lifting a given weight by a given height (Carnot, 1824)
  - ▶ think of a gas inside a piston
    - ★ the amount of **work** required to move the piston such that we change the volume by a small amount  $dV$  is proportional to the pressure that opposes moving it

$$dW = -P dV$$

- ▶ Above turns out to work for any **reversible** process in a **closed** system.
- Conservation of energy

$$dU = \delta Q - P dV$$

# Original concept of entropy

- Carnot recognised that in any physical process there were losses
  - ▶ tendency to dissipate **useful** energy
  - ▶ often appears as heat
- Clausius (1850s)
  - ▶ heat flows from hot to cold
  - ▶ gave the dissipated heat a name: entropy and a formula

$$dS = \frac{\delta Q}{T}$$

- Boltzmann and Gibbs gave it a statistical basis

# Comments

- All of the above is grossly over-simplified
  - ▶ no chemistry
    - ★ no interactions
    - ★ molecules as rigid spheres
  - ▶ no quantum mechanics
  - ▶ not much mathematics
- But we need a context to talk about entropy WRT statistical mechanics

## Section 2

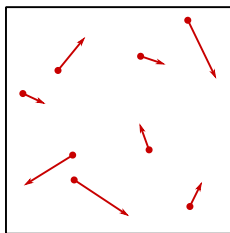
# Physics and Statistical Mechanics



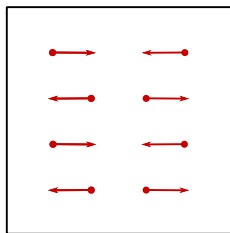
# What did we miss?

- Macro-state

- ▶ given a particular temperature, the particles could be random, or organised



random



organised

- ▶ Pressure, temperature, volume,  $n$  can all be the same for both, but there is an important difference
  - ★ ideal gas assumes random
  - ★ macroscopic properties didn't capture this

- Might be “obvious” to use entropy somehow here?

# Equilibrium again

The fundamental assumption of thermodynamics is that given no information to the contrary we assume that in equilibrium all possible microstates are equally likely.

- The same as Laplace's principle of indifference
  - ▶ the arguments for it are essentially the same, plus
  - ▶ Liouville's Theorem helps
- Remember that this space includes all velocities as well as positions
  - ▶ but there can be constraints implied by macroscopic quantities
    - ★ e.g., temperature implies some (at least statistical) limit on velocities
  - ▶ so what we work towards is actually maximum entropy, i.e., at equilibrium, the entropy will be maximised while observing any constraints

# Entropy (Boltzmann)

- Given above assumptions, entropy is

$$S = -k \sum_i p_i \ln p_i = k \ln |\Omega|$$

- ▶  $k$  is a constant (remember we had an arbitrary constant in entropy before, which implicitly set the units)
- ▶ in physics

$$k = k_B = 1.38065 \times 10^{-23} \text{ J/degree K}$$

which is [Boltzmann's constant](#)

# Microcanonical ensemble

- Assume we have an isolated system in equilibrium
  - ▶ for example an ideal gas
  - ▶ equilibrium implies macroscopic variables are fixed:  $N, V, T$
  - ▶ in turn, energy  $E$  is fixed

We call this system the **microcanonical ensemble**.

- We can approximately calculate  $|\Omega|$ 
  - ▶ ideal gas  $U = E$ , the kinetic energy
  - ▶ momentum of atom is  $\mathbf{p}_i$

$$E = \sum_{i=1}^n \frac{\|\mathbf{p}_i\|^2}{2m}$$

- ▶ fixing this is like specifying points must be on the surface of a  $3n$ -dimensional hyper-sphere radius  $r = \sqrt{2mE}$
- ▶ number of possible states  $\simeq$  surface area
- ▶ also number of states for  $\mathbf{x}_i$  is  $\propto V$

$$|\Omega| \propto (2mE)^{n/2} V^n$$

- But particles are identical, so  $n!$  states are indistinguishable

# Microcanonical ensemble

- Assume we have an isolated system in equilibrium
  - ▶ for example an ideal gas
  - ▶ equilibrium implies macroscopic variables are fixed:  $N$ ,  $V$ ,  $T$
  - ▶ in turn, energy  $E$  is fixed

We call this system the **microcanonical ensemble**.

- We can approximately calculate entropy

$$\begin{aligned} S(E) &= k_B \ln |\Omega| \\ &\simeq k_B n \ln \left[ \frac{\pi(4\pi mE)^{3/2} V}{3h^3 n^2} \right] + \frac{5}{2} k_B n \end{aligned}$$

- ▶ note approximate linear dependence on  $n$
- ▶ note also

$$\frac{\partial S}{\partial E} = \frac{3nk_B}{2E} = \frac{1}{T}$$

which essentially gives us back Clausius' relationship.

# Microcanonical ensemble

- Assume we have an isolated system in equilibrium
  - ▶ for example an ideal gas
  - ▶ equilibrium implies macroscopic variables are fixed:  $N$ ,  $V$ ,  $T$
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We call this system the **microcanonical ensemble**.

- Maximum entropy distribution for particles with given mean energy
  - ▶ implies exponential distribution of energy of individual particles
  - ▶ in physics, this is names the **Boltzmann distribution**, and might be written

$$n_i \propto \exp\left(-\frac{U_i}{k_B T}\right)$$

where  $n_i$  is the number of particles at energy  $U_i$

- ▶ from this we could get the Maxwell-Boltzmann distribution for the speeds of the particles
- ▶ it applies more widely than just the ideal gas

# Thought Experiment 1

- Take two gases in separate chambers
- Open a door between them so they can mix until they reach equilibrium
- Energy, mass, and volume are conserved so

$$E = E_1 + E_2$$

$$N = N_1 + N_2$$

$$V = V_1 + V_2$$

- Temperature  $T = \frac{2E}{3k_b n} \propto E/N$  so

$$T = c \frac{E}{N} = c \frac{E_1 + E_2}{N_1 + N_2} = \frac{N_1 T_1 + N_2 T_2}{N_1 + N_2}$$

so temperature is a weighted mean of original temperatures.

# Thought Experiment 1

- What about entropy?
  - ▶ define per particle entropy

$$s(E) = \lim_{n \rightarrow \infty} \frac{S(nE)}{n}$$

- The “volume” of the new phase space

$$|\Omega(N_1 E_1 + N_2 E_2)| \geq |\Omega(N_1 E_1)| \times |\Omega(N_2 E_2)|$$

- So resulting (per particle) entropy

$$\begin{aligned} s(N_1 E_1 + N_2 E_2) &\simeq \frac{k \ln |\Omega(N_1 E_1 + N_2 E_2)|}{N_1 + N_2} \\ &= \frac{k \ln |\Omega(N_1 E_1)|}{N_1 + N_2} + \frac{k \ln |\Omega(N_2 E_2)|}{N_1 + N_2} \\ &\geq \frac{N_1}{N_1 + N_2} \frac{k \ln |\Omega(N_1 E_1)|}{N_1} + \frac{N_2}{N_1 + N_2} \frac{k \ln |\Omega(N_2 E_2)|}{N_2} \\ &\simeq \lambda_1 s(N_1 E_1) + \lambda_2 s(N_2 E_2) \end{aligned}$$



# Law's of Thermodynamics

- 1 Conservation of energy (energy can't be created or destroyed, only shifted around)
  - ▶ i.e., you can't win
- 2 Entropy increases (as an isolated system evolves, some energy is lost to “randomness” or heat, and this increase over time)
  - ▶ you can't break even
- 3 You can't get to absolute zero (zero entropy)
  - ▶ you can't get out of the game

# Maxwell's demon

- Imagine a “demon” sitting in the doorway between two chambers
- He chooses which particles to allow through the door
- Only allows “hot” fast particles through to the right, and “cold” slow particles to the left
- Right heats up, and left cools
- Reverses entropy

# Further reading I



Thomas M. Cover and Joy A. Thomas, *Elements of information theory*, John Wiley and Sons, 1991.



Neri Merhav, *Information theory and statistical physics – lecture notes*, arXiv: 1006.1565v1, June 2010.