

Information Theory and Networks

Lecture 32: Information Theory, the Universe and Everything

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Lecture_notes/InformationTheory/](http://www.maths.adelaide.edu.au/matthew.roughan/Lecture_notes/InformationTheory/)

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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

1 mole is essentially defined by the constant, but its origin was the number of molecules in 32g of oxygen.

In an ideal gas there are no particle rotations or vibrations, so the energy of the particles is just the "translational" kinetic energy.

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

In other problems macro-state might include other features, e.g.,

- magnetic or electrostatic field strength (which might be variable WRT to position)
- flow rate either of fluid, or charge (e.g., current), or some other property
- for a solid: colour, reflectivity, transparency, hardness, conductivity (of heat or charge)

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.



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Remember: absolute temperature in Kelvins:

- absolute zero means all particles have stopped
- water freezes (at surface pressure) at about 273 K

Note, in all of the above, we ignore bulk motion of the system as a whole (e.g. in calculating kinetic energy).

Also, Newton's laws imply equal and opposite forces: so we can think of pressure as the force exerted on the gas to keep it in a constant volume, or (perhaps more correctly) as the force of the gas on its container.

Average is given by temperature, but at any one instant, the proportion of particles moving at a given speed within this range is determined by probability as described by the MaxwellBoltzmann distribution.

We can see the movement of individual particles as Brownian motion (as was originally done in experiments).

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, ...



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Doesn't include everything (some properties are neither).

Also, implies independence between components, as otherwise phenomena such a volume might not be extensive (e.g. imagine combining two chemicals that react).

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"

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Thermodynamic equilibrium encompasses a lot of other cases: e.g. two systems at

- thermal equilibrium are at same temperature
- mechanical equilibrium are at same pressure
- etc.

Are systems really ever in such a state – only approximately.

Zerth law seems to be to create mathematical ordering or structure to the "temperature" as a variable. i.e., that it is one-dimensional, or that $T_1 > T_2$ has absolute meaning, and similarly for other macroscopic variables.

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

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If we do the work slowly enough, Adiabatic theorem suggests that the system will stay in approximately equilibrium states, so we don't have to worry about jumps in system energy. But some transitions we consider allow for jumps (e.g., opening a door between two regions), and the implicit assumption in most thermodynamics is that the number of particles is large enough that we reach equilibrium again very quickly.

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
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Heat and temperature are extensive and intensive versions of the same thing.

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

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

- ΔQ is heat added (or lost)
- ΔW is work done on the system
 - e.g., by changing the pressure
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- This is the 1st law of thermodynamics

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Obviously, the above is a simplification, e.g., assumes the system is closed and can exchange only heat and work.

For example, when we add heat to a system (say a gas in a balloon) some may result in a raised temperature, but some may do work which increases the volume of the balloon.

So work is being implicitly defined by the relationship above, which essentially comes down to conservation of energy. Some heat energy becomes internal energy and some work (or visa versa).

Implicitly, this defines the direction of work as energy flow from the working system to the surroundings (energy transfers to the system are considered positive).

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

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

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Work of lifting a weight to given height is proportional to weight and height.

Can also have work without a change of volume (isochoric work), say by stirring. Joule (1845) ran a paddle wheel in an insulated barrel that was turned by a falling weight, and the increase in heat in the water was measured.

Meaning of

$$dW = -P dV$$

is really that

$$W = \int_{V_1}^{V_2} P dV$$

but where use of δ there is a path dependence in integrals.

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

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Note that although we can get useful work out of heat, we can only do so if there is a differential, e.g., two bodies at different temperatures. Uniform heat isn't exploitable.

S is the symbol used for entropy in physics.

- extensive (proportional to size of system)
- relative (need to have some bench mark to set it up, so $S = 0$ for absolute zero, perfect crystal)

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

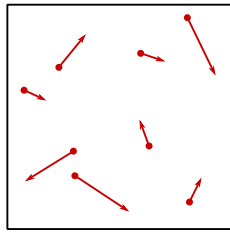
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Section 2

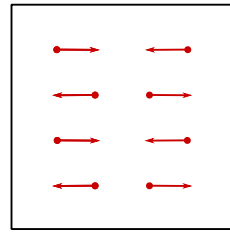
Physics and Statistical Mechanics

What did we miss?

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



random

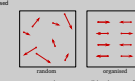


organised

- ▶ 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?



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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



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Liouville's theorem asserts that the density of points in the vicinity of a point travelling through the phase-space of a system is constant in time (for a Hamiltonian system), so if the distribution is uniform at some time, it remains so.

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

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$|\Omega|$ is the number of states, which will obviously be huge here, and by uniformity assumption $p_i = 1/|\Omega|$.

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

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An ensemble is a collection of possible states with a probability distribution over those states.

n is the number of particles (remember N was this number but with units of moles).

Results from [Mer10], and see also the Sackur-Tetrode equation http://en.wikipedia.org/wiki/Sackur-Tetrode_equation and http://en.wikipedia.org/wiki/Gibbs_paradox

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$$S(E) = k_B \ln |\Omega|$$

$$\simeq k_B n \ln \left[\frac{\pi(4\pi mE)^{3/2} V}{3h^3 n^2} \right] + \frac{5}{2} k_B n$$

- 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.

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Stirling's approximation

$$\ln(n!) \simeq n \ln n$$

Linear dependence makes it an extensive quantity.

Note that this requires an implicit definition of temperature

$$T = \frac{2E}{3k_B n}$$

which relates to the ideal gas law by

$$PV = NRT = nk_B T$$

so Boltzmann's constant is the scaled version of the idea gas constant.

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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

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Exponential distribution was proved to be max entropy distribution with constant mean (in previous lecture).

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

$$\begin{aligned} E &= E_1 + E_2 \\ N &= N_1 + N_2 \\ V &= V_1 + V_2 \end{aligned}$$

- 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.



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- 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

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



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So entropy increases, and it turns out this is actually a general law, called the 2nd law of thermodynamics.

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

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- You can't get to absolute zero (zero entropy)
 - you can't get out of the game


There is a notional zeroth law that sets the scene: "if two systems are both in thermal equilibrium with a third system then they are in thermal equilibrium with each other". Essentially it establishes the notion of temperature as something meaningful.


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

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Further reading I

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

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