Information as a physical entity, entropy and life
@ Complexity Explorers Kraków

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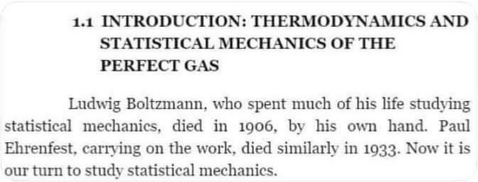
December 5, 2019

Outline

Thermodynamics

Based on [3].



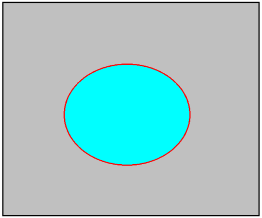
1.1 INTRODUCTION: THERMODYNAMICS AND STATISTICAL MECHANICS OF THE PERFECT GAS

Ludwig Boltzmann, who spent much of his life studying statistical mechanics, died in 1906, by his own hand. Paul Ehrenfest, carrying on the work, died similarly in 1933. Now it is our turn to study statistical mechanics.

Figure: Goodstein, 'States of Matter'

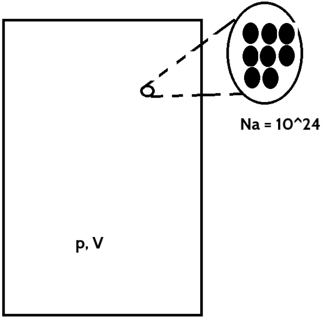
System

We identify some system from the environment by distinguishing some more or less formal boundaries with some specific physical properties (e.g., heat contact or permeability of particles). Such a system should be macroscopically uniform in the sense of its physical and chemical properties - a so-called *simple system*.



System

By practical reasons (or if we do not know that atoms exist), we reduce a large degree of freedom to only a few.



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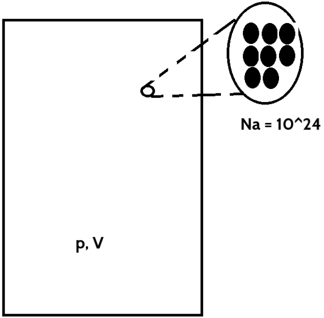
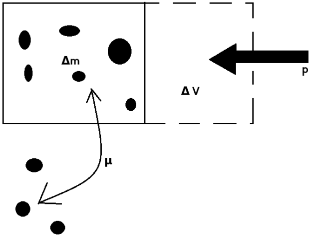


So is there any additional variable that can point out a direction of behaviour of the system left on its own?

Energy change

- We want to be extremely practical and minimalistic. Lets identify how energy flows between system and environment.
- Work: It is always some kind of 'external force'(F) times the displacement Δr generated by this work: $W = F \times \Delta r$, e.g.,
  - $p \times \Delta V$ - pressure p induces change in volume V;
  - $\mu \times \Delta m$ - each particle changing mass by Δm carries some energy μ;
  - ...
- Is there any other way to transmit energy?



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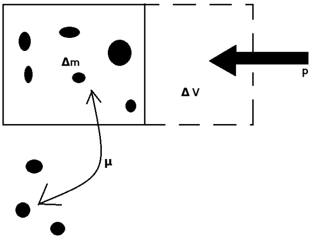

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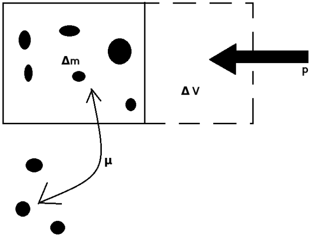

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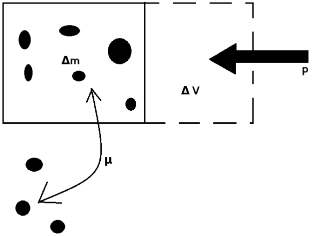

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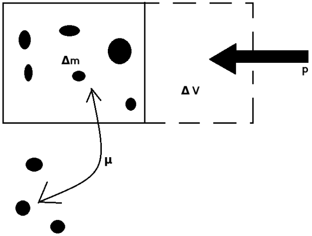

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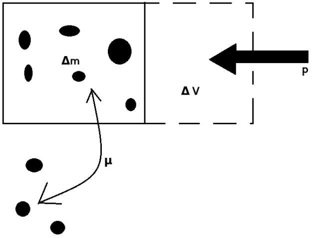

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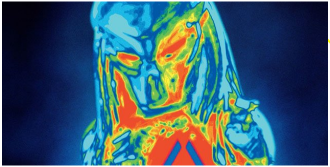

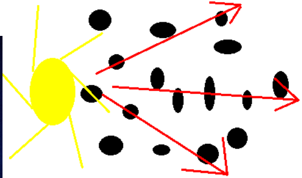

Figure: Right, scene from 'Predators' movie.

The equivalence of heat and work was observed by Julius Robert von Mayer, who noticed the change of the blood colour of sailors under various geographic longitudes.

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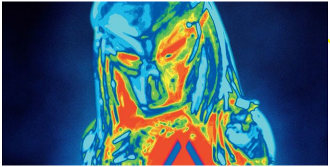

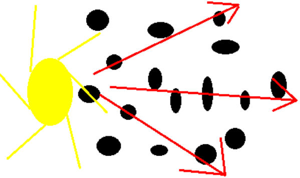

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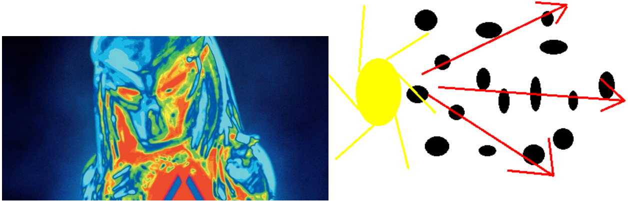

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Processes

Process in Thermodynamics

- A process is a change of state $x \to y$.
- A *quasi-static* process is represented as a path in a state space.
- A *non-quasi-static* process cannot be represented as a path in a state space.
- An *adiabatic quasi-static* process $Q = 0$ (change along the path).
- An *adiabatic non-quasi-static* process Q and W has no sense since there is no path in a state space. $U(x) - U(y)$ has sense.

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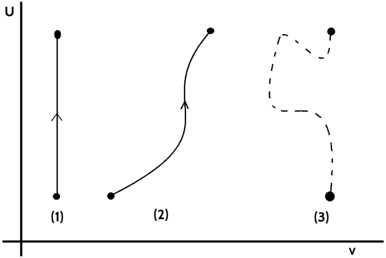

- (1) - heating at constant volume $W = 0$, $\Delta U = Q$,
- (2) - quasi-static adiabatic process $Q = 0$, $\Delta U = -W$,
- (3) - stirring at constant volume, adiabatic but not quasi-static (no curve in a state space).

Energy balance vel The First Law of Thermodynamics

Lets do the budget of energy:

$$\text{Internal change of energy} = \pm\text{Heat transfer} + \pm\text{Work done}$$

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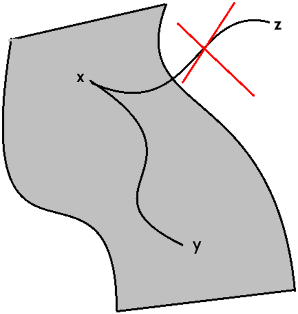
If we leave the system isolated (adiabatically), can it change arbitrary? NO! The system changes only in certain directions.



How about car paring?

Figure: Can we move slightly right using only forward-backward-turn motions? From https://debo2pt.files.wordpress.com/2013/10/parking.jpg

How about car paring?

Figure: Yes! We Can! From https://i.pinimg.com/originals/f0/a9/e2/f0a9e2cb7524dd88e4f6c18d1841aceb.jpg

All is in constraints.

- Car parking is **nonholonomic constraint** - all possible moves allows us to explore whole available space.
- The Second Law of Thermodynamics is **holonomic constraint** - we must move along some prescribed curves/surfaces in space.

For gifted amatours: This is a particular statement of Frobenius theorem on the integrability of distribution (directions): When all possible moves allows us to explore whole space, and when to explore some smaller parts only.

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Entropy

This (holonomic) constraint is entropy S, and we can write (via Frobenius theorem $Q \wedge dQ = 0$):

$$Q = T\Delta S, \tag{2}$$

where T is the temperature (longer story).

The Second Law of Thermodynamics again

The Second Law of Thermodynamics (Caratheodory)

In every neighbourhood of every state x there are states y that are not accessible from x via **quasi-static adiabatic** paths (along which $Q = 0$).

We have alternative formulations (no necessary equivalent):

Second Law of Thermodynamics (Kelvin)

In quasi-static cyclic process a quantity of heat cannot be converted entirely into its mechanical equivalent of work.

Second Law of Thermodynamics - Corollary: 'Entropy increases'

If a state y results from x by any adiabatic process (quasi-static or not), then $S(y) \geq S(x)$.

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Second Law of Thermodynamics - Corollary: Entropy increases

If a state y results from x by any adiabatic process (quasi-static or not), then $S(y) \geq S(x)$.

In other words: in a system and environment the change of entropy is always non-negative!!!

Lets state it precise for interested people:

- There is a contact space defined by the 1-form: $\theta := dU - TdS + pdV - \mu dm$.
- Thermodynamical system is described by maximal(Legendre) submanifold Φ such that the First Law of Thermodynamics holds: $\Phi^*\theta = 0$.
- The Second Law of Thermodynamics: Q defines globally foliation of the contact space. The leafs of foliations are defined by the constant entropy.
- The Third Law of Thermodynamics is outside of thermodynamics: for $T = 0$ we have $S = 0$ - it fixes the scale of entropy.
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Figure: Figure from Mike Pauken, 'Thermodynamics for Dummies', John Wiley & Sons, 2011

Entropy, chaos and life

"The general struggle for existence of animate beings is not a struggle for raw materials – these, for organisms, are air, water and soil, all abundantly available – nor for energy which exists in plenty in any body in the form of heat, but a struggle for [negative] entropy, which becomes available through the transition of energy from the hot sun to the cold earth." L. Boltzmann, *The second law of thermodynamics* (Theoretical physics and philosophical problems). Springer-Verlag New York, LLC.

"Let me say first, that if I had been catering for them [physicists] alone I should have let the discussion turn on free energy instead. It is the more familiar notion in this context. But this highly technical term seemed linguistically too near to energy for making the average reader alive to the contrast between the two things." Erwin Schrödinger, *What is Life?*, 1944

Entropy vs Chaos

What about ordering and its connection to entropy?

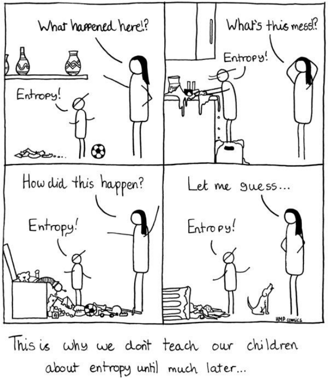

Figure: From
https://www.pinterest.com/pin/248894316882821824/.

The magic of entropy

High entropy (or increase of it) is USUALLY visible as increase of chaos... However the biochemical compounds of living organisms have entropy not drastically bigger than chaotic mixture of its constituent atoms [6].

Lets see what we have inside:

- Your Body's Molecular Machines: https://www.youtube.com/watch?v=X_tYrnv_o6A
- Electron Transport Chain: https://www.youtube.com/watch?v=rdF3mnyS1p0
- How Enzymes Work: https://www.youtube.com/watch?v=yk14dOOvwMk

Lets explain it in some details.

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Open systems

Figure: Open, Closed and Isolated system. Which is which? From https://x-engineer.org/graduate-engineering/signals-systems/control-systems/the-concept-of-system-in-engineering/.

Open systems and (bio)chemical reactions

Increase of total entropy ΔS_{tot} is equal to the increase of the entropy of the system ΔS_{sys} and the environment ΔS_{env}. It should be nonegative according to The Second Law:

$$\Delta S_{sys} + \Delta S_{env} = \Delta S_{tot} \geq 0. \quad (3)$$

Assume that the system and environment is in the constant temperature T. Define:

- Enthalpy change (dispersed heat): $\Delta H_{sys} := -T\Delta S_{sys} = (T\Delta S_{env})$.
- Gibbs free energy change: $\Delta G = -T\Delta S_{tot}$.

Then we have:

$$\Delta G = \Delta H_{sys} - T\Delta S_{sys}. \quad (4)$$

Now the Second Law is:

$$\Delta G \leq 0. \quad (5)$$

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Assume that the system and environment is in the constant temperature T. Define:

- Enthalpy change (dispersed heat): $\Delta H_{sys} := -T\Delta S_{sys} = (T\Delta S_{env})$.
- Gibbs free energy change: $\Delta G = -T\Delta S_{tot}$.

Then we have:

$$\Delta G = \Delta H_{sys} - T\Delta S_{sys}. \tag{4}$$

Now the Second Law is:

$$\Delta G < 0. \tag{5}$$

Open systems and (bio)chemical reactions

$$\Delta G = \Delta H_{sys} - T\Delta S_{sys}. \quad (6)$$

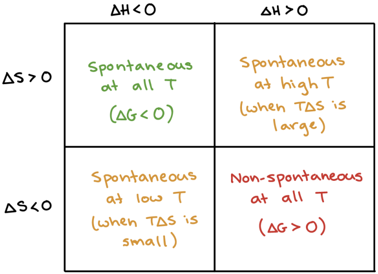

Figure: That is why Schrodinger talked about Enthalpy. From https://www.khanacademy.org/science/chemistry/thermodynamics-chemistry/gibbs-free-energy/a/gibbs-free-energy-and-spontaneity

Maxwell's Demon

Figure: Photo from
https://www.flickr.com/photos/uaart/4582135868/

Simplified experiment

- Consider a single particle of ideal gas in a box (Szilard 30').
- The particle is in thermal equilibrium with thermostat(box) of temperature T.
- We will try to extract work from this system in a cycle.
- Let's start the cycle...

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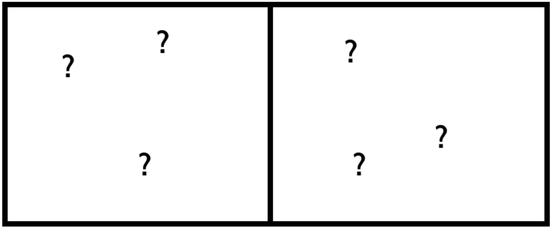

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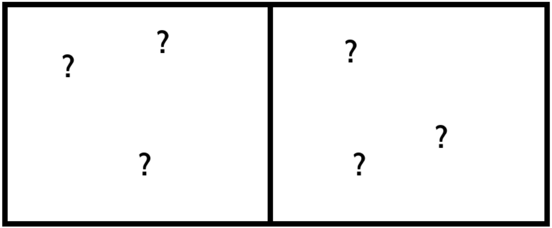

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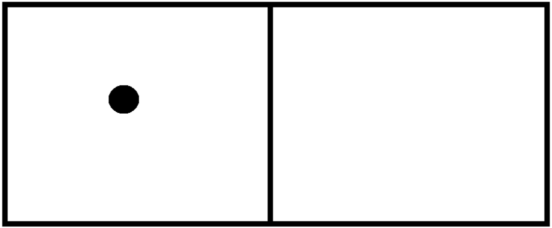
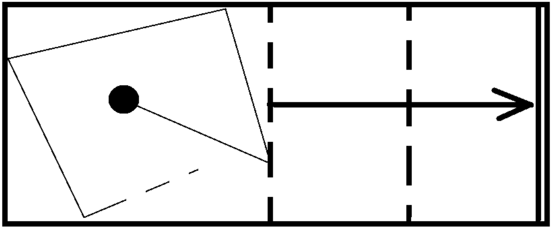
Where is the particle?



We localize the particle, so we can use it to extract work.

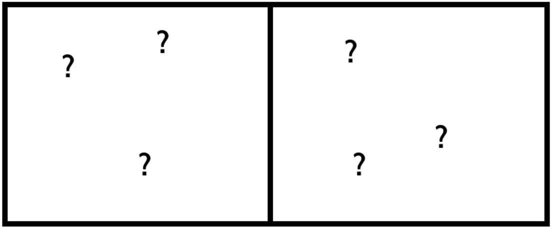
Extract work



The work extracted in adiabatic expansion is (state equation $pV = k_B T$):

$$W = k_B T \int_{V/2}^{V} \frac{dV}{V} = k_B T \ln(2). \tag{7}$$

Repeat



So we returned to the beginning extracting only some work $W = k_B T \ln(2)$.

What Thermodynamics says about this situation?

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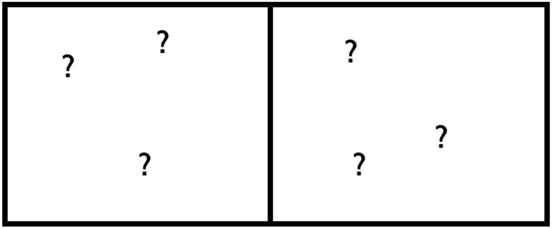

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Second Law of Thermodynamics

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What Thermodynamics says about this situation?

- No single heat source can be used to construct heat engine - heater must be used and some heat expelled.
- The change of entropy of system (heater S_H) and universe (cooler S_C) must be non-negative: $\Delta S = S_C - S_H \geq 0 \quad \rightarrow \quad S_H = \frac{Q_H}{T} = \frac{W}{T} \leq S_C$, i.e.,

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Landauer's principle

Figure: Photo from https://www.natureindex.com/article/10.1103/physrevlett.120.020601

- Landauer (70s, @IBM) associated the irreversible memory operation (e.g. deletion) with emission of $Q \geq k_B T \ln(2)$ per bit.
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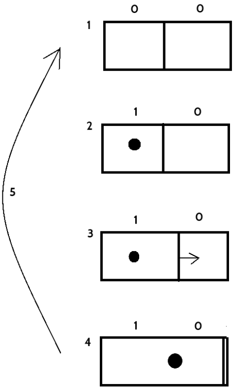

- The work done in $3 \to 4$ is $W = k_B T \ln(2)$.
- The (Landauer's) heat emitted in 5 is $Q \geq k_B T \ln(2)$.
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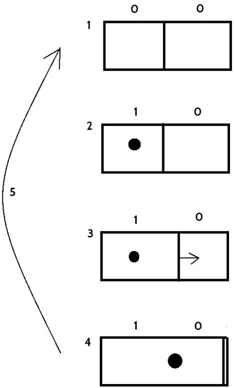

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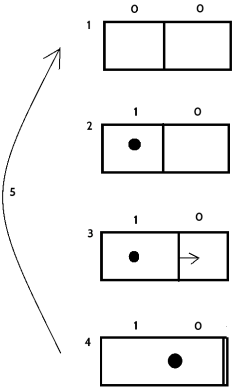

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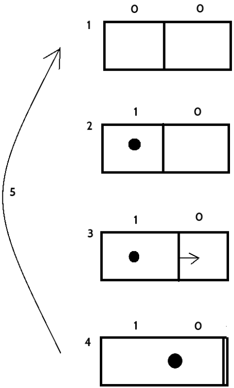

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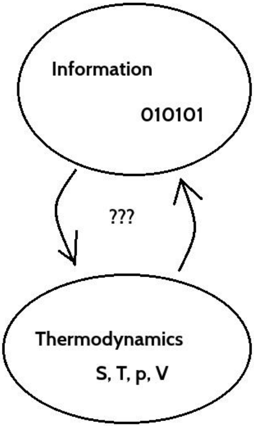
Abstract approach

Q: Assuming Landauer's principle, is information 'level' somehow separated from its physical realization?



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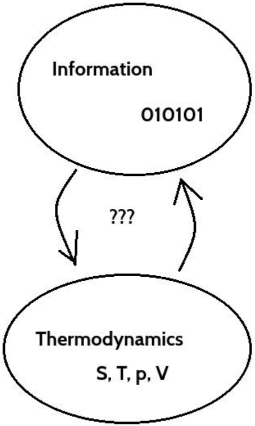

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Entropy and Ordering

Based on [1].

Adiabatic accessibility

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Y is adiabatically accessible from X, ($X \prec Y$) when there is an adiabatic process that transforms X into Y.

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Properties of ordering

- Monotonicity: $X \sim X$
- Transitivity: $X \prec Y$ and $Y \prec Z$ then $X \prec Z$
- Consistency: $X \prec X'$ and $Y \prec Y'$ implies $(X, Y) \prec (X', Y')$
- Scaling invariance: $\lambda > 0$ and $X \prec Y$ implies $\lambda X \prec \lambda Y$
- Splitting recombination: $X \sim (\lambda X, (1 - \lambda) X)$
- Stability: if $(X, \epsilon Z) \prec (Y, \epsilon Z')$ then $X \prec Y$ for $\epsilon \to 0^+$.

The ordering is a 'pullback' of ordering from the ordering of the real numbers...

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$S : \Gamma \to \mathcal{R}$ is called entropy if it fulfills

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Entropy

Theorem 4 [1]

The relation $\prec$ defines uniquely entropy S up to multiplicative and additive constant.

Crash course in category theory

There are two types of people at parties:

- Set-theorists - judge person on clothes (s)he wears.
- Category-theorists - judge person on how (s)he interacts with others.

V.L.

Figure: https://www.eventbrite.co.uk/blog/throw-an-epic-party-ds00/

Basic notation

Category

Category $\mathcal{C}$ consist of two kinds of elements

- objects denoted by $A, B, C, \ldots$;
- morphisms(arrows, maps) between objects, denoted by $f, g, h, \ldots$;
- Arrows fulfils:
  - Composition: If $A \xrightarrow{f} B$ and $B \xrightarrow{g} C$, then $A \xrightarrow{g \circ f} C$.
  - Associativity: $(f \circ g) \circ h = f \circ (g \circ h)$.
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Category Set

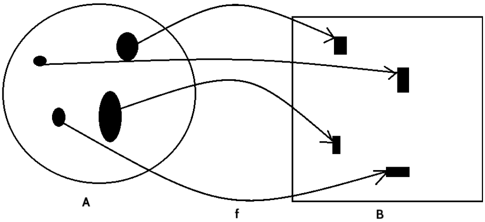


Figure: Category Set.

Left and right inverse

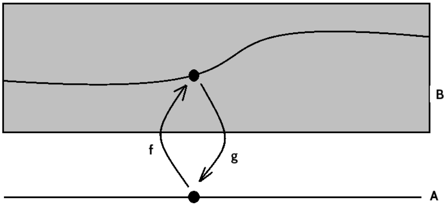
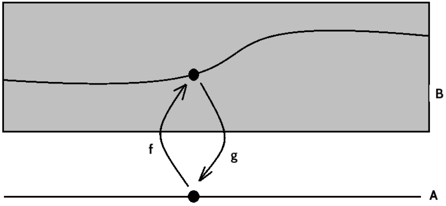


Figure: If $g \circ f = 1$ then f is left inverse (section) and g is called right inverse (retraction). Which set has less points?

Q: When also $f \circ g = 1$?
Ans: When A and B will have 'the same number of points'. Then f is inverse to $g = f^{-1}$.

Left and right inverse



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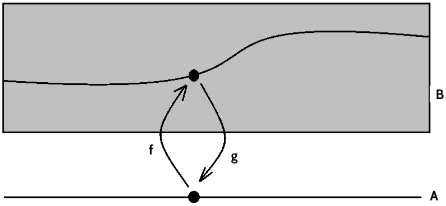

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Functors

Functor maps between different categories. It maps objects to corresponding objects and arrows to corresponding arrows.

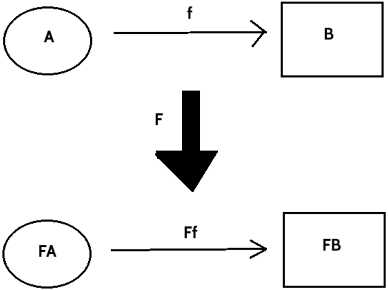
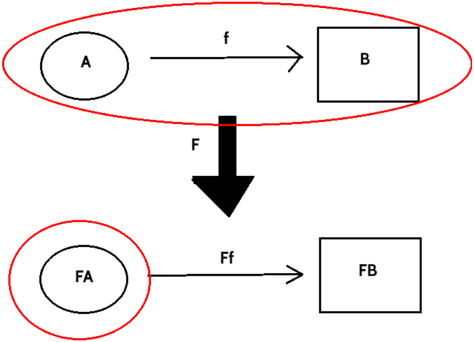


Figure: Schematic representation of functor.

Functors and Haskell

Lets look on functor in a different way.



$$fmap :: (Functor F) \Longrightarrow (a \rightarrow b) \rightarrow Fa \rightarrow Fb$$

(Take a function $f : a \rightarrow b$ and initial data Fa and map it to Fb.)

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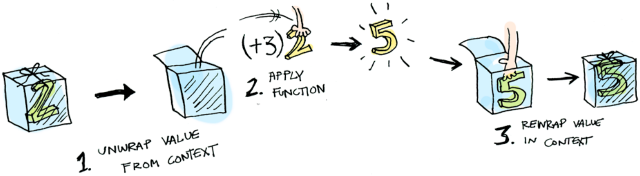

Figure: That is how Haskell functors act. This mechanism of wrapping data into context helps to isolate functional from non-functional world in Monads. From http://adit.io/posts/2013-04-17-functors,_applicatives,_and_monads_in_pictures.html

Array as a functor:

instance Functor [] where

fmap = map

Application:

fmap (+3) [1..3]

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Poset

Poset (partially ordered set) is a set P with partial order $\prec$. The arrow $x \to y$ for $x, y \in P$ exists iff $x \prec y$.

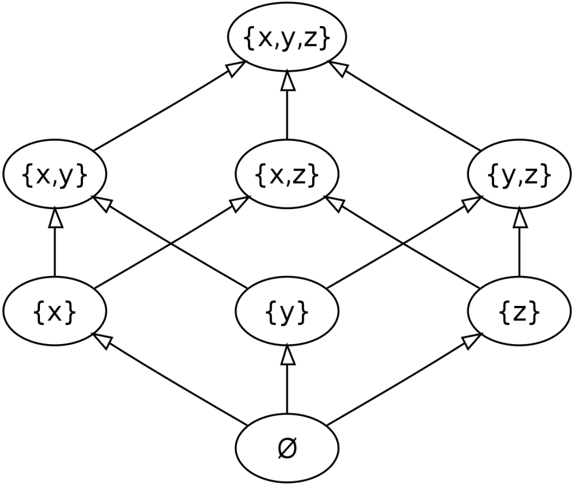

Figure: An example of Poset with inclusion as ordering, from Wikipedia.

Monotone map

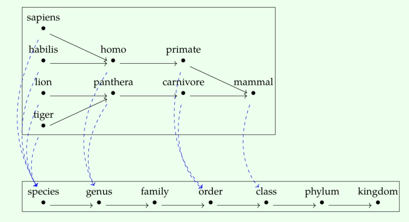

Figure: Example of order preserving functor(map): if $x \to y$ then $Fx \to Fy$. From [5].

Order-preserving mappings

Let $\mathcal{C} = (C, \preccurlyeq)$ and $\mathcal{D} = (D, \sqsubseteq)$ are two posets then the mapping (functor) $F : \mathcal{C} \to \mathcal{D}$ is

- *monotone* if for any $x, y \in C$, if $x \preccurlyeq y$, then $Fx \sqsubseteq Fy$;
- *order-embedding* if for all $x, y \in C$, $x \preccurlyeq y \Leftrightarrow Fx \sqsubseteq Fy$;
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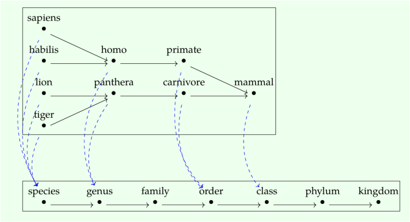

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Galois connection - an example of Adjoin functors

Galois connection

A Galois connection between preorders P and Q is a pair of monotone maps $f : P \to Q$ and $g : Q \to P$ such that

$$f(p) \leq q \Leftrightarrow p \leq g(q). \tag{9}$$

We say that f is the left adjoint and g is the right adjoint of the Galois connection.

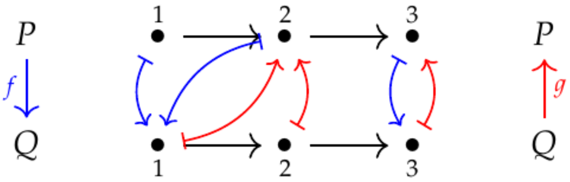

Figure: Example of Galois connection [5].

Galois connection - an example of Adjoin functors

The most illuminating example - theory and model:

- set of theories - ordered by finer details;
- set of models that realize theories - ordered by details of realization;
- The Galois connection 'realizes' implementation of theory on model, and abstraction of theory from model;

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Entropy in category theory

See [2].

The Plan

1. state-space (G-Set) + entropy $\rightarrow$ total ordering,
2. total ordering $\rightarrow$ poset (G-poset) structure,
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Ladnauer's functors

Entropy system

The *entropy system* is the object of G-Pos category, which objects are $\mathcal{G} = (\Gamma, \preccurlyeq)$, with preserving ordering group $(\mathbb{R}^+, \cdot, 1)$ action, where the (partial or) total order is given by the entropy function $S : \Gamma \to \mathbb{R}$.

Galois connection in terms of entropy

Entropy system $\mathcal{G}_1 = (\Gamma_1, S_1)$ is implemented/realized/simulated in the entropy system $\mathcal{G}_2 = (\Gamma_2, S_2)$ when there is a Galois connection between them, namely, there is a functor $F : \mathcal{G}_1 \to \mathcal{G}_2$ and a functor $G : \mathcal{G}_2 \to \mathcal{G}_1$ such that $F \dashv G$. The condition for Galois connection:

$$S_2(Fc) \leq S_2(d) \Leftrightarrow S_1(c) \leq S_1(Gd). \tag{10}$$

We name the functors F and G the Landauer's functors.

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Processes

Adiabatic reversible/irreversible processes

An entropy system map, that is a poset map $f : \Gamma \to \Gamma$ is reversible at $p \in \Gamma$, if $p = f(p)$, that is $S(p) = S(f(p))$, i.e. f at p preserves entropy. Otherwise f is irreversible at p.

Note:

- This is definition for ANY poset which is induced from 'entropy' structure.
- It should work for any system, not necessary thermodynamic one.

Main Theorem

For two entropy systems $\mathcal{G}_1 = (\Gamma_1, \preccurlyeq)$ and $\mathcal{G}_2 = (\Gamma_2, \sqsubseteq)$, and functors $F : \mathcal{G}_1 \to \mathcal{G}_2$ and $G : \mathcal{G}_2 \to \mathcal{G}_1$, we have following possibilities for Landauer-Galois' connections

1. for which $F \dashv G$,

Possibilities	Γ_2 reversible	Γ_2 irreversible
Γ_1 reversible	YES	YES
Γ_1 irreversible	NO	YES

2. transpose above table for $G \dashv F$,
3. for which F, G are

Possibilities	Γ_2 reversible	Γ_2 irreversible
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order-embeddings; If the functors are surjective, then they are order-isomorphisms.

Main Theorem

In short:

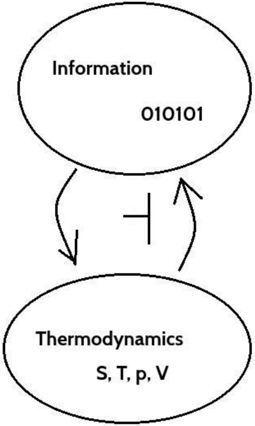

Figure: $\dashv$ is the Galois connection.

Applications

See [2].

Toy example [2, 5]

- Two systems: $\Gamma_1 = (\mathbb{R}_{\geqslant 0}, S)$ and $\Gamma_2 = (\mathbb{N}_{\geqslant 0}, S)$ with $S(x) = x$.
- Consider $F : \Gamma_1 \to \Gamma_2$ defined as $F(z) = \lceil \frac{z}{3} \rceil$ and $G : \Gamma_2 \to \Gamma_1$ given by $G(z) = 3z$.
- We have obviously $F \dashv G$, i.e.

$$\left\lceil \frac{x}{3} \right\rceil \leq y \quad \Leftrightarrow \quad x \leq 3y. \tag{11}$$

  - Take $f : \Gamma_1 \to \Gamma_1$ given by a simple shift $f(z) = z + 0.2$.
    Irreversibility of f at $x = 1$: $S(x) = 1$. Then $\bar{x} = f(x) = 1.2$ and $S(f(x)) = 1.2$.
    Reversibility of image map: $y = F(x) = 1$ with $S(y) = 1$, and $\bar{y} = F(\bar{x}) = Ff(\bar{x}) = 1$ with $S(\bar{y}) = 1$
  - If we take $f(x) = x$ then reversible (trivial) process in Γ_1 is mapped to reversible process in Γ_2.
  - No irreversible process in Γ_2 can be realized by a reversible process in Γ_1.
- We restored $F \dashv G$ case from The Main Theorem.

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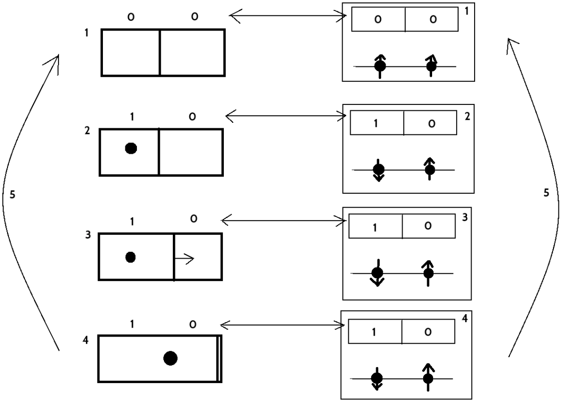
Landuauer's explanation of Maxwell's Demon



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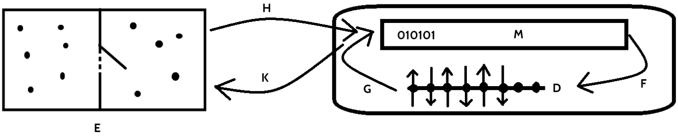
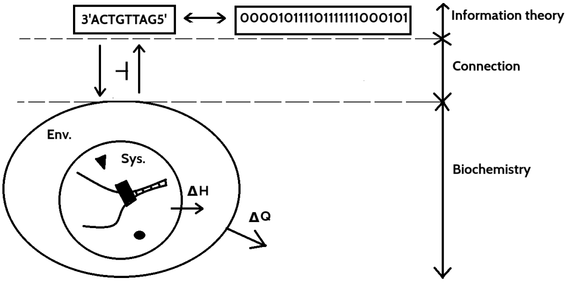
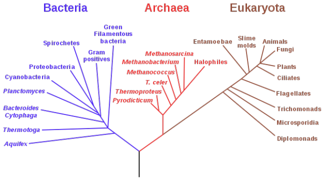


DNA computing



Evolution



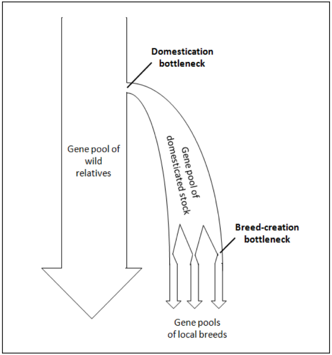


Figure: Tree of life vs gene pool. Left `https://futurism.com/theres-revised-tree-life-1000-new-species`, right `http://scientificbeekeeping.com/whats-happening-to-the-bees-part-4-the-genetic-consequences-of-`

Evolution [5, 2]

- $(P, \subseteq)$ - population with $p \subseteq q$ if the animal species p is also the animal species q in the sense of specificity on the Tree of life;
- $(G, \leq)$ describes gene polls and the ordering has the following meaning: $a \leq b$ when the gene pool b can be generated by the gene pool a.
- $i : P \to G$ sends each population to the gene pool that defines it.
- $cl : G \to P$ sends each gene pool to the set of animals that can be obtained by recombination of the given gene pool.
- $i \dashv cl$
- Reversing the process, we can define entropy of genes and populations. We can even define Landauer's heat of evolution.

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Thank You for Your Attention

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