Foundations of Entropy II

Let's calculate 'em

Lecture series at the

School on Information, Noise, and Physics of Life

Nis 19.-30. September 2022

by Jan Korbel

all slides can be found at: **slides.com/jankorbel**

Activity II

You have 3 minutes to write down on a piece of paper:

What is the most unexpected/surprising application
of **entropy**
you have seen? (unexpected field, unexpected result)

Entropy-based Adaptive Sampling

Jaume Rigau Miquel Feixas Mateu Sbert
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Universitat de Girona, Catalonia, Spain

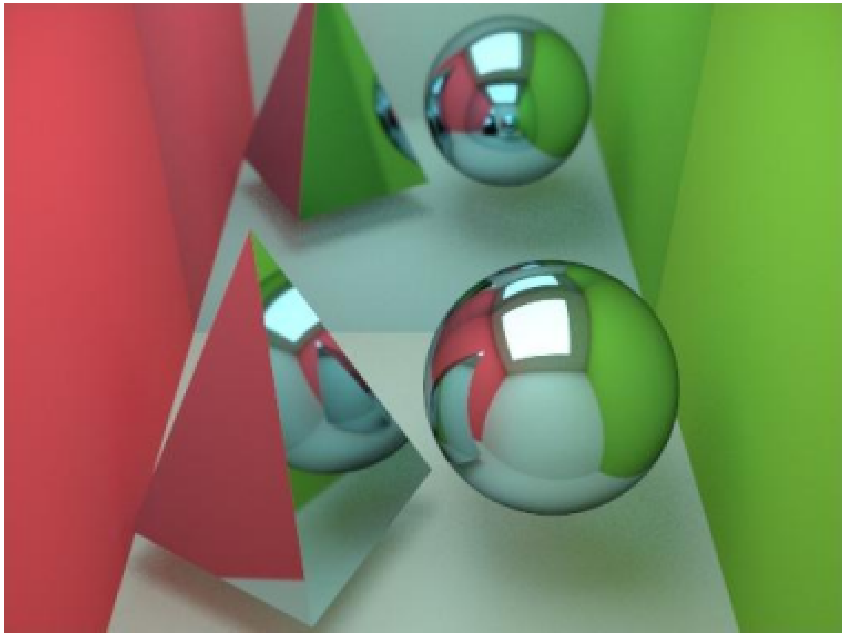

Figure 4: Reference image used in the test in Figure 5 with 1024 rays per pixel.

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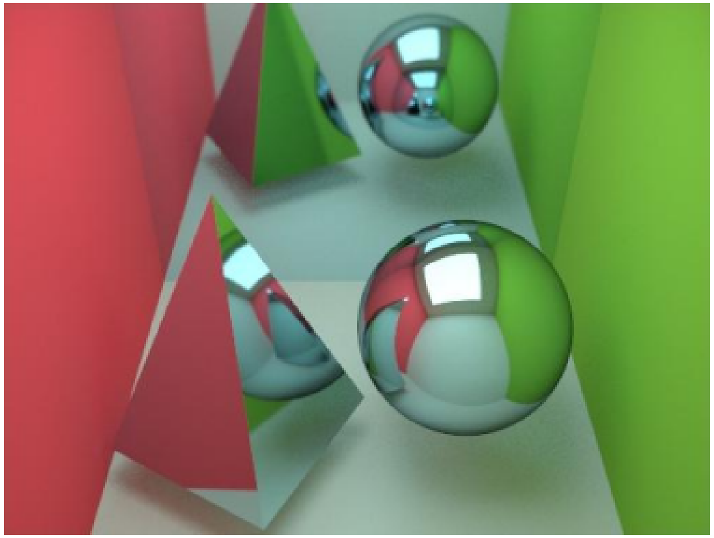


Figure 4: Reference image used in the test in Figure 5 with 1024 rays per pixel.

Using Boltzmann's formula for non-multinomial systems

As we saw in the previous lecture, the multinomial multiplicity

$$W(n_1, \ldots, n_k) = \binom{n}{n_1, \ldots, n_k}$$

leads to Boltzmann-Gibbs-Shannon entropy.

Are there systems with non-multinomial multiplicity?

What is their entropy?

Ex. I: MB, FD & BE statistics

1. Maxwell-Boltzmann statistics - N distinguishable particles, N_i particles in state ϵ_i

Multiplicity can be calculated as

$$W(N_1, \dots, N_k) = \binom{N}{N_1}\binom{N-N_1}{N_2}\dots\binom{N-\sum_{i=1}^{k-1} N_1}{N_k} = N! \prod_{i=1}^{k} \frac{1}{N_i!}$$

If ϵ_i has degeneracy g_i, then

$$W(N_1, \dots, N_k) = N! \prod_{i=1}^{k} \frac{g_i^{N_i}}{N_i!}$$

Then, we get

$$\boxed{S_{MB} = -N \sum_{i=1}^{k} p_i \log \frac{p_i}{g_i}}$$

Ex. I: MB, FD & BE statistics

2. Bose-Einstein statistics - N indistinguishable particles, N_i particles in state ϵ_i with degeneracy g_i,

Multiplicity can be calculated as

$$W(N_1, \ldots, N_k) = \prod_{i=1}^{k} \binom{N_i + g_i - 1}{N_i} \qquad (|*)$$

Let us introduce $\alpha_i = g_i/N$. Then, we get

$$\boxed{S_{BE} = N \sum_{i=1}^{k} \left[(\alpha_i + p_i)\log(\alpha_i + p_i) - \alpha_i \log \alpha_i - p_i \log p_i\right]}$$

Ex. I: MB, FD & BE statistics

3. Fermi-Dirac statistics - N indistinguishable particles, N_i particles in state ϵ_i with degeneracy g_i, maximally 1 particle per sub-level (thus $N_i \leq g_i$)

Multiplicity can be calculated as

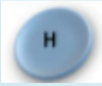
$$W(N_1, \ldots, N_k) = \prod_{i=1}^{k} \binom{g_i}{N_i}$$

Let us introduce $\alpha_i = g_i/N$. Then, we get

$$\boxed{S_{FD} = N \sum_{i=1}^{k} \left[-(\alpha_i - p_i) \log(\alpha_i - p_i) + \alpha_i \log \alpha_i - p_i \log p_i \right]}$$

Ex. II: structure-forming systems

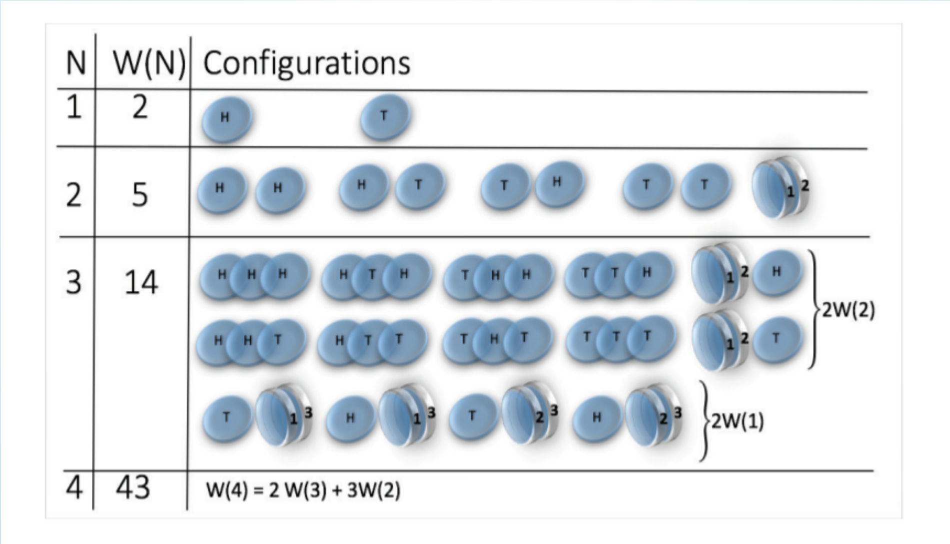
Let us start with a simple example of a coin tossing.

States are:  

But! let's make a small change, we consider *magnetic coins*

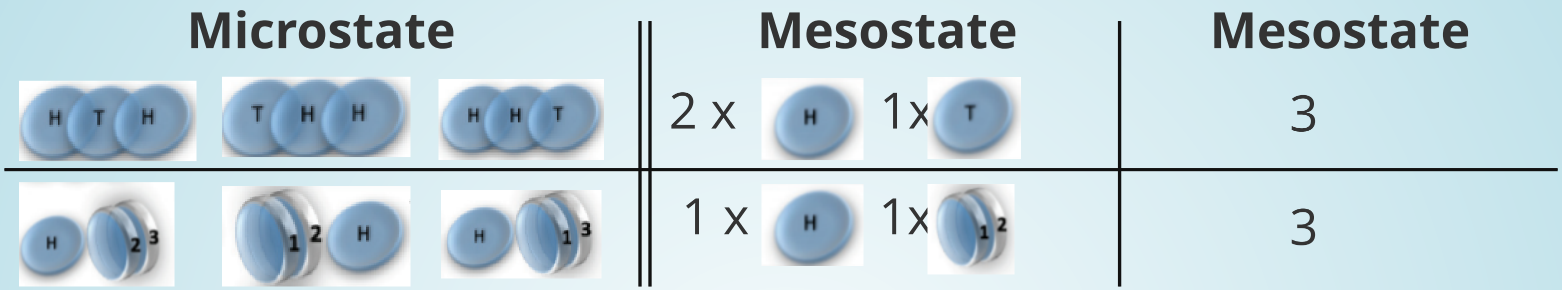
The bound (or sticky) state is simply 

State space grows super-exponentially $(W(n) \sim n^n \sim e^{n \log n})$

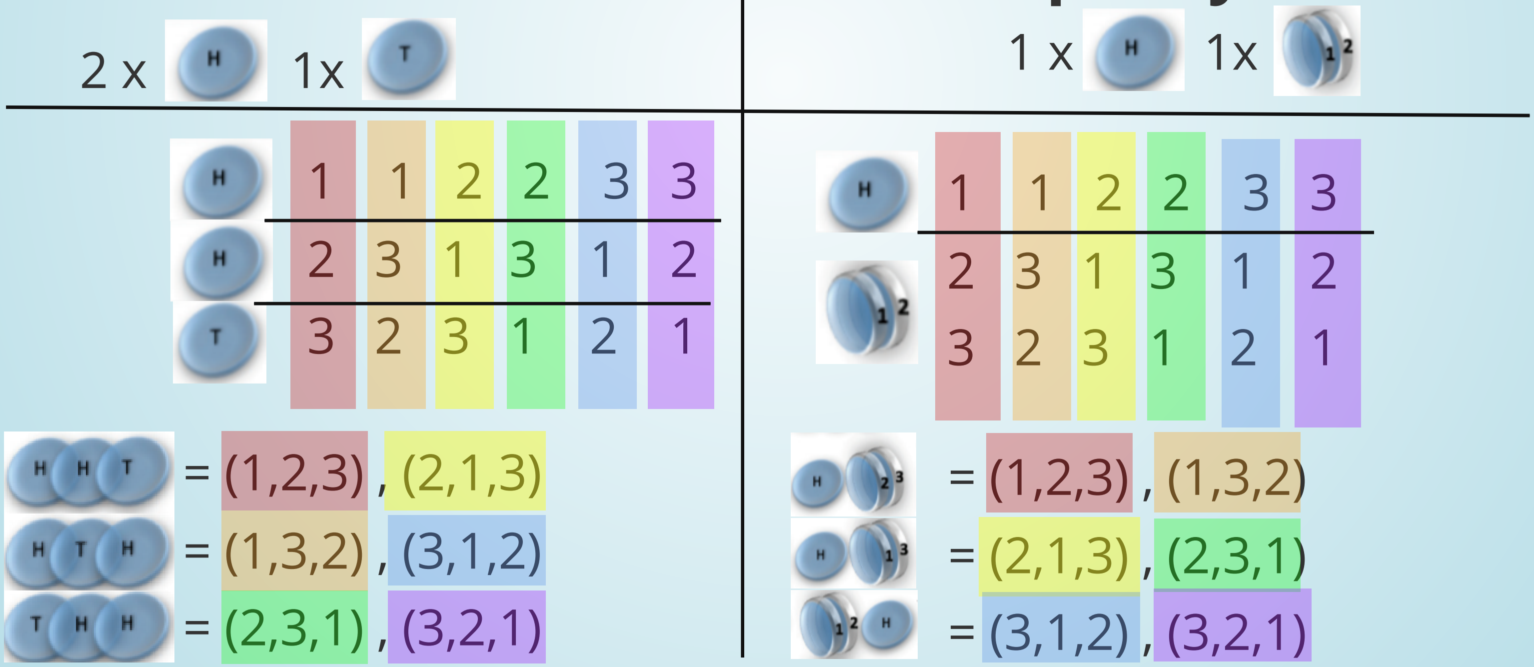


picture taken from: Jensen et al 2018 J. Phys. A: Math. Theor. 51 375002

Multiplicity

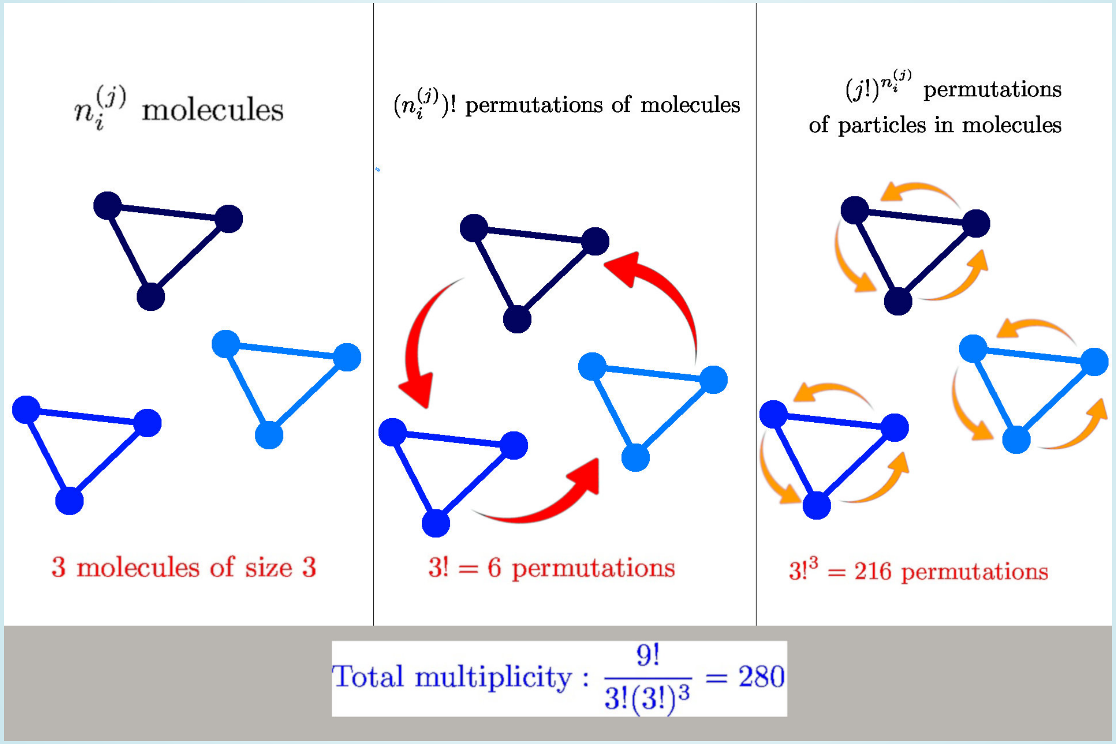


How to calculate multiplicity



Multiplicity

we have $n_i^{(j)}$ molecules of size j in a state $s_i^{(j)}$



General formula: $W(n_i^{(j)}) = \dfrac{n!}{\prod_{ij} n_i^{(j)}!\,(j!)^{n_i^{(j)}}}$

Boltzmann's 1884 paper

III. ***Ueber das Arbeitsquantum, welches bei chemischen Verbindungen gewonnen werden kann; von Ludwig Boltzmann in Graz.***

(Aus dem 88. Bde. der Sitzungsber. der k. Akad. der Wiss. zu Wien, II. Abth. vom 18. Oct. 1883 mitgetheilt vom Hrn. Verf.)

Es seien z. B. A Chlor- und B Wasserstoffatome gegeben. Es wird gefragt, wie wahrscheinlich es ist, dass sich daraus gerade N_1 Chlor-, N_2 Wasserstoff- und N_3 Chlorwasserstoffmolecüle bilden. Hier ist $a_1 = 2$, $b_1 = 0$; $a_2 = 0$, $b_2 = 2$; $a_3 = 1$, $b_3 = 1$; die Anzahl der Chloratome ist $A = 2N_1 + N_3$; die Anzahl der Wasserstoffatome ist $B = 2N_2 + N_3$: die Anzahl der Bildungsweisen:

$$\boxed{Z = \frac{A!\,B!}{2^{N_1+N_2}\,.\,N_1!\,N_2!\,N_3!}}$$

Entropy of structure-forming systems

$$S = \log W \approx n \log n - \sum_{ij} \left(n_i^{(j)} \log n_i^{(j)} - n_i^{(j)} + n_i^{(j)} \log j! \right)$$

Introduce "probabilities" $\wp_i^{(j)} = n_i^{(j)}/n$

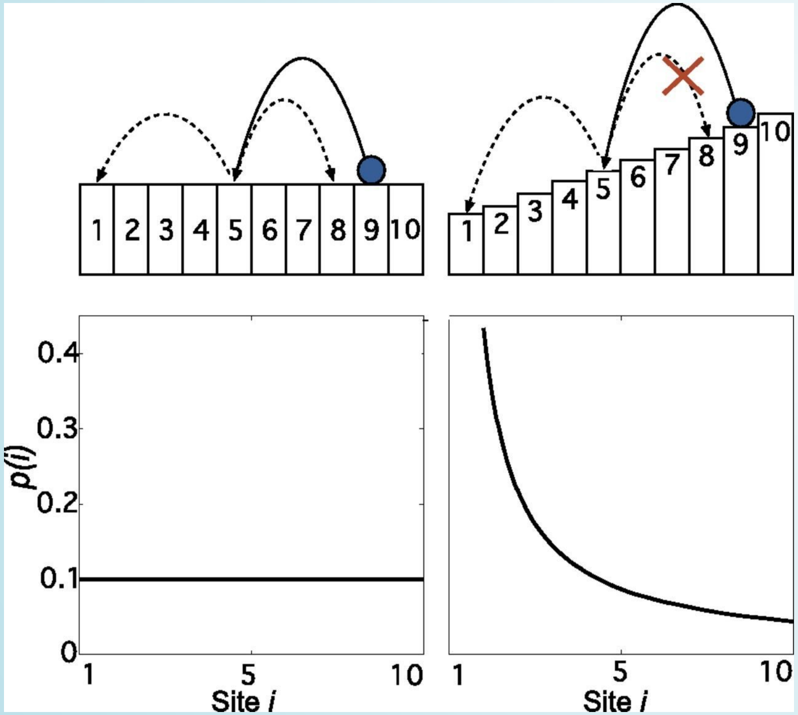
$$\mathcal{S} = S/n = -\sum_{ij} \wp_i^{(j)} (\log \wp_i^{(j)} - 1) - \sum_{ij} \wp_i^{(j)} \log \frac{j!}{n^{j-1}}$$

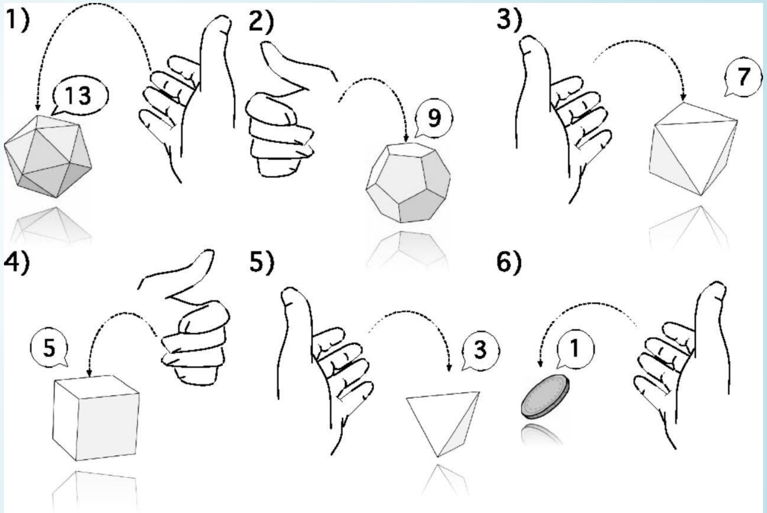
Finite interaction range: concentration $c = n/b$

$$\boxed{\mathcal{S} = S/n = -\sum_{ij} \wp_i^{(j)} (\log \wp_i^{(j)} - 1) - \sum_{ij} \wp_i^{(j)} \log \frac{j!}{c^{j-1}}}$$

Nat. Comm. 12 (2021) 1127

Ex. III: sample-space reducing processes (SSR)





Corominas Murtra, Hanel, Thurner *PNAS* 112(17) (2015) 5348

Multiplicity

The number of states is n. Let us denote the states as $x_n \to \cdots \to x_1$, where x_1 is the ground state, where the process restarts. Let us sample R relaxation sequences $x = (x_{k_1}, \ldots, x_1)$.

The sequences can be visualised as

$r \times i$	W	$W-1$	$W-2$	$\cdots$	2	1
1	$*$	$-$	$-$	$\cdots$	$*$	$*$
2	$-$	$*$	$*$	$\cdots$	$-$	$*$
3	$*$	$-$	$*$	$\cdots$	$-$	$*$
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
$R-2$	$-$	$*$	$*$	$\cdots$	$-$	$*$
$R-1$	$-$	$*$	$-$	$\cdots$	$*$	$*$
R	$-$	$-$	$*$	$\cdots$	$-$	$*$
	k_W	k_{W-1}	k_{W-2}	$\cdots$	k_2	k_1

Each run must contain x_1

How many of these sequences contain a state x_j exactly k_j times?

Multiplicity

Number or runs $R \equiv k_1$, number of them containing x_j is k_j

Multiplicity of these sequences: $\binom{k_1}{k_j}$

By multiplying the multiplicity for each state we get

$$W(k_1, \ldots, k_n) = \prod_{j=2}^{n} \binom{k_1}{k_j}$$

$$\log W \approx \sum_{j=2}^{n} [k_1 \log k_1 - \cancel{k_1} - k_j \log k_j + \cancel{k_j} - (k_1 - k_j) \log(k_1 - k_j) + \cancel{(k_1 - k_j)}]$$

$$\approx \sum_{j=2}^{n} \left[k_1 \log k_1 - k_j \log k_1 - k_j log \frac{k_j}{k_1} - (k_1 - k_j) \log(k_1 - k_j)\right]$$

By introducing $p_i = k_i / N$ where N is the total number of steps, we get

$$\boxed{S_{SSR}(p) = -N \sum_{j=2}^{n} \left[p_i \log\left(\frac{p_i}{p_1}\right) + (p_1 - p_i) \log\left(1 - \frac{p_i}{p_1}\right)\right]}$$

Ex. IV: Pólya urns

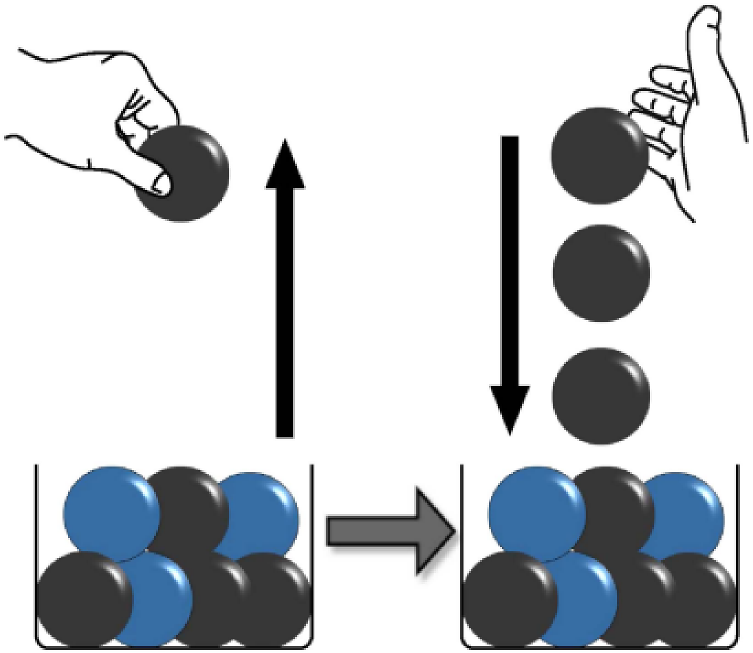


Figure 1. Schematic illustration of a Pólya process. When a ball of a certain color is drawn, it is replaced by $1+\delta$ balls of the same color. Then the next ball is drawn and the process is repeated for N iterations. Here $\delta=2$. This reinforcement process creates a history-dependent dynamics. The configurations obtained after successive iterations have non-multinomial structure.

Hanel, Corominas Murtra, Thurner New J. Phys. (2017) 19 033008

Probability of a sequence

We have c colors, initially $n_i(0) \equiv n_i$ balls of color c_i. After a ball is drawn, we return δ balls of the same color to the urn.

After N draws, the number of balls in the urn is

$$n_i(N) = n_i + \delta k_i$$

where k_i is the number of draws of color c_i. The total number of balls is $n(R) = \sum_c n_c(N) = N + \delta N$

The probability of drawing a ball of color c_i in N-th run, is $p_i(N) = n_i(N)/n(N)$. The probability of sequence $\mathcal{I} = \{i_1, \ldots, i_N\}$ is

$$\boxed{p(\mathcal{I}) = \prod_{j=1}^{c} \frac{n_j^{(\delta,k_j)}}{n^{(\delta,N)}}}$$

where $m^{(\delta,r)} = m(m+\delta)\ldots(m+r\delta)$

Probability of a histogram

A histogram $\mathcal{K} = \{k_1, \ldots, k_c\}$ is defined as $k_c = \sum_{j=1}^{N} \delta(i_j, c)$

Thus the probability of observing a histogram is

$$\boxed{p(\mathcal{K}) = \binom{N}{k_1, \ldots, k_c} p(\mathcal{I})}$$

$$n_j^{(\delta,k_j)} \approx k_j! \delta^{k_j} \; (k_i + 1)^{n_i/\delta}$$

$$p(\mathcal{K}) = \frac{N!}{\prod_{j=1}^{c} \cancel{k_j!}} \frac{\prod_{j=1}^{c} \cancel{k_j!} \delta^{k_j} \, (k_j+1)^{n_j/\delta}}{n^{(\delta,N)}}$$

... technical calculation ...

$$\boxed{S_{Pólya}(p) = \log p(\mathcal{K}) \approx -\sum_{i=1}^{c} \log(p_i + 1/N)}$$

Ex. IV: q-deformations

This example is rather theoretical, but provides us a useful hint of what happens if there are correlations in the sample space

Motivation: finite versions of $\exp$ and $\log$

$\exp(x) = \lim_{n \to \infty} \left(1 + \frac{x}{n}\right)^n$

So define

$\exp_q(x) := (1 + (1-q)x)^{1/(1-q)}$

$\log_q(x) := \frac{x^{1-q} - 1}{1-q}$

Let us find an operation s.t.

$\exp_q(x) \otimes_q \exp_q(y) \equiv \exp_q(x+y)$

$\Rightarrow a \otimes_q b = \left[a^{1-q} + b^{1-q} - 1\right]^{1/(1-q)}$

Suyari, Physica A 368 (2006) 63-82

Calculus of q-deformations

In analogy to $n! = 1 \cdot 2 \cdot \dots \cdot n$ introduce $n!_q := 1 \otimes_q 2 \otimes_q \ \cdots \otimes_q n$

It is than easy to show that $\log_q n!_q = \frac{\sum_{k=1}^n k^{1-q} - n}{1-q}$ which can be used for generalized Stirling's approximation $\log_q n!_q \approx \frac{n}{2-q} \log_q n$

Let us now consider a q-deformed multinomial factor

$$\binom{n}{n_1, \dots, n_k}_q := n!_q \oslash_q (n_1!_q \otimes_q \cdots \otimes_q n_k!_q)$$

$$= \left[\sum_{l=1}^{n} l^{1-q} - \sum_{i_1}^{n_1} i_i^{1-q} - \cdots - \sum_{i_k}^{n_k} i_k^{1-q} \right]^{1/(1-q)}$$

Tsallis entropy

Let us consider that the multiplicity is given by a q-multinomial factor $W(n_1, \ldots, n_k) = \binom{n}{n_1, \ldots, n_k}_q$

In this case, it is more convenient to define entropy as $S = \log_q W$, which gives us:

$$\boxed{\log_q W = \frac{n^{2-q}}{2-q} \frac{\sum_{i=1}^k p_i^{2-q} - 1}{q-1} = \frac{n^{2-q}}{2-q} S_{2-q}(p)}$$

This entropy is known as **Tsallis entropy**

Note that the prefactor is not n but n^{2-q}

(*non-extensivity)* - we will discuss this later

Entropy and energy

Until now, we have been just counting states; let us now discuss the relation with **energy**.

We consider that the states describe the energy of the system (either Hamiltonian or more generalized energy functional)

Therefore, entropy is defined as

$$S(E) := \log W(E)$$

Ensembles

There are a few typical situations:

1. Isolated system = microcanonical ensemble

Let $H(s)$ be the energy of a state s. Multiplicity is then

$$\boxed{W(E) = \sum_s \delta(H(s) - E)}$$

Phenomena like negative "temperature" $T = \frac{\mathrm{d}S(E)}{\mathrm{d}E} < 0$

2. closed system = canonical ensemble

Total system is composed of the system of interest (S) and the heat reservoir/bath (B). They are weakly coupled i.e., $H_{tot}(s, b) = H_S(s) + H_B(b)$ (no interaction energy)

$$W(E_{tot}) = \sum_{s,b} \delta(H_{tot}(s, b) - E_{tot})$$

3. open system = grandcanonical ensemble

Entropy in canonical ensemble

This can be further rewritten as

$$= \int \mathrm{d}E_S \sum_s \delta(H_S(s) - E_S) \sum_b (H_B(b) - (E_{tot} - E_S))$$

$$= \int \mathrm{d}E_S \, W_S(E_S) W_B(E_{tot} - E_S)$$

This is hard to calculate. Typically, the dominant contribution is from the maximal configuration of the integrand, which we obtain from

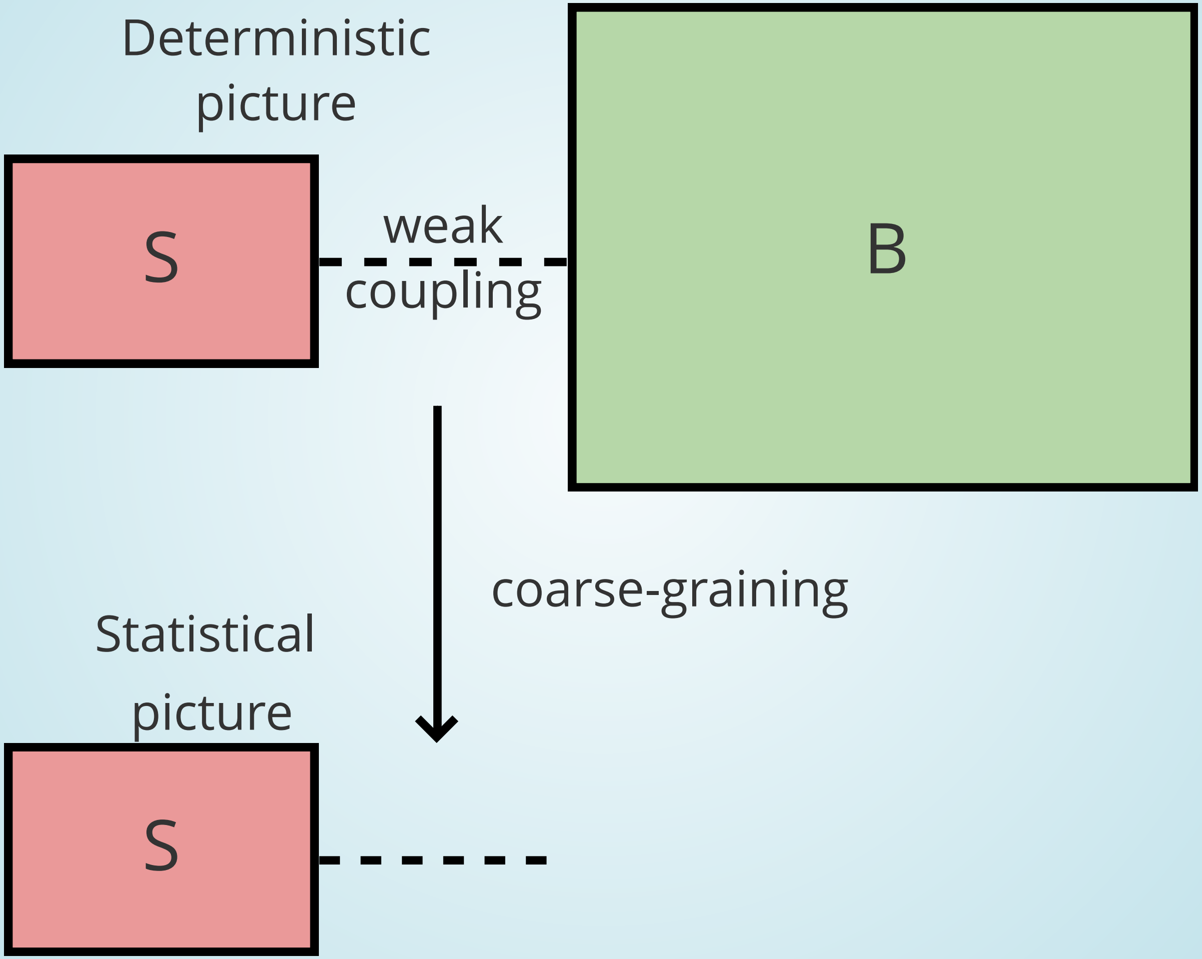
$$\frac{\partial W_S(E_S) W_B(E_{tot} - E_S)}{\partial E_S} \stackrel{!}{=} 0 \Rightarrow \frac{W_S'(E_S)}{W_S(E)} = \frac{W_B'(E_{tot} - E_S)}{W_B(E_{tot} - E_S)}$$

As a consequence $\frac{\partial S_E(E_S)}{\partial E_S} \stackrel{!}{=} \frac{\partial S_B(E_{tot} - E_S)}{\partial E_S} := \frac{1}{k_B T}$

and $\underbrace{S_B(E_{tot} - E_S)}_{free\ entropy} = \underbrace{S_B(E_{tot})}_{bath\ entropy} - \frac{\partial S}{\partial E_S} E_S + \dots$

This is the emergence of **Maximum entropy principle**

Canonical ensemble & Coarse-graining



Summary