



Thermodynamics Beyond Molecules

Thermodynamics and the Evolution of Populations

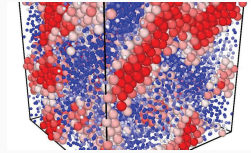
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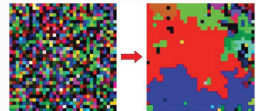
International Conference on Thermodynamics 2.0
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- Thermodynamics is a *universal* language. What does this mean?
- The impulse to apply thermodynamics to all sort of problems is undeniable. What drives this *intuitive urge*?
- What are the rules for applying thermodynamics outside *physics*?
- To *export* thermodynamics to the non-physical world we must *separate* it from physics. Is that even possible?
- What *is* thermodynamics?



<https://phys.org/news/2018-03-glass-transition-driven-thermodynamics.html>



Sociophysics. Physics Today 71, 2, 40 (2018); doi: 10.1063/PT.3.3845



<https://physicsworld.com/a/the-social-physics-of-voting-behaviour/>



Our goal is to:

- *Deconstruct* thermodynamics
- *Throw* physics away
- *Reconstruct* “thermodynamics” without physics

Thermodynamic entropy



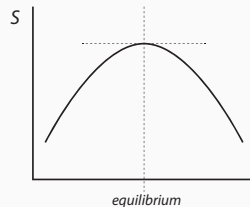
Before Boltzmann and Gibbs thermodynamics was about *heat* and *work* and its main question was to *maximize* the amount of work in a cycle. This is a variational problem and it is answered by the *maximization of the entropy*:



$$\max S(E, V, N)$$

Entropy function: elusive but computable.

$$S(E, V, N) = \int \frac{dQ_{\text{rev}}}{T}$$





With *Boltzmann* and *Gibbs* entropy becomes a *functional* of a probability distribution:

$$S[p] = - \sum_i p_i \log p_i$$

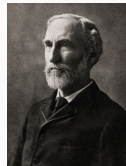
The equilibrium distribution maximizes the entropy functional among all feasible probability distributions that can be assigned to a set of microstates:

$$p^* : \quad S[p^*] \geq S[p]; \quad p \in \mathcal{E}_{X,Y \dots}$$

A *feasible* distribution is one that satisfies all macroscopic specifications of state $(X, Y \dots)$.



Ludwig Boltzmann



J. Willard Gibbs

How Statistical Thermodynamics Works



In the canonical ensemble $(\bar{E}, V, N)$ the set $\mathcal{E}$ of *feasible* distributions is all distributions that satisfy

$$\sum_i p_i = 1, \quad \sum_i E_i p_i = \bar{E}$$

The variational problem is to maximize $-\sum_i p_i \log p_i$ under the constraints of the feasible set and the solution is

$$p_i^* = \frac{e^{-\beta E_i}}{Q(\beta)}, \quad (1)$$

with

$$\bar{E} = -\frac{\partial \log Q}{\partial \beta} \quad (2)$$

$$\Omega(E) = \log Q - \beta \bar{E} \quad (3)$$

$$\beta = \frac{\partial \log \Omega(\bar{E})}{\partial \bar{E}} \quad (4)$$

Where is *physics* in these results???



Shannon obtained the entropy functional by means unrelated to physics. Shannon's entropy is a measure of *uncertainty*. The canonical probability distribution has the maximum uncertainty among all distributions with the same mean.



Claude Shannon

Jaynes took this further:

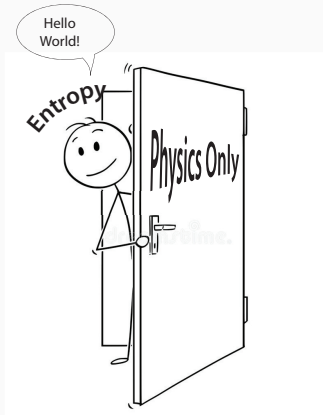
[w may have now reached a state where statistical mechanics is no longer dependent on physical hypotheses, but may become simply an example of statistical inference (Jaynes, 1957)]



E. T. Jaynes



Shannon unlocked the door and Jaynes kicked it open.
Entropy has escaped!



But where does it go from here?

Random Sampling



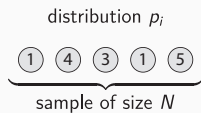
Start with a *generic* probability distribution $P(X = x_i) = q_i$ and collect a *random sample* $(n_1, n_2 \cdots n_N)$ of size N . Form the intensive empirical distribution of the sample $p_i = n_i/N$. The probability to obtain $\{p\}$ is

$$P(\{p\}) = N! \prod_i \frac{q_i^{n_i}}{n_i!}$$

Take the log:

$$\frac{\log P(\{p\})}{N} = - \sum_i p_i \log \frac{p_i}{q_i}$$

The *Most Probable Distribution* of the empirical sample is the distribution that is being sampled $\{p\}$.



distribution q_i

Biased Sampling



Bias the selection of the sample by a homogeneous functional W :

$$\log W(\{p\}) = \sum_i \frac{\partial \log W(\{p\})}{\partial p_i}$$

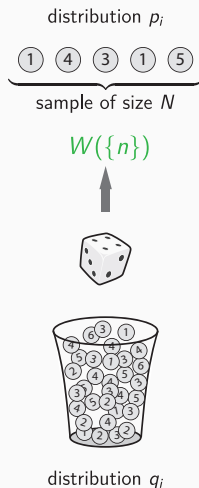
The probability to obtain distribution $\{p\}$ in the sample is

$$\frac{\log P(\{p\})}{N} = - \sum_i p_i \log \frac{p_i}{w_i q_i} - \log(\text{norm.})$$

Most Probable Distribution:

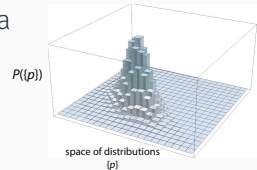
$$p_i^* = w_i \frac{p_i}{r}$$

Setting $w_i = f_i/p_i$, **any** distribution f_i becomes the Most Probable Distribution





- Biased sampling from any probability distribution $\{q\}$ establishes a *space of distributions* $\{p\}$ in the same domain and a *probability measure* $P(\{p\})$.
- By proper selection of the the bias, *any* distribution in this space can be obtained as the Most Probable Distribution.
- When the sample size is large the Most Probable Distribution is *overwhelmingly more probable* than all others.





Draw biased samples from the *exponential distribution*

$$q_i = \frac{e^{-x_i/\bar{x}}}{\bar{x}}$$

The probability of empirical distribution $\{p\}$ is

$$\frac{\log P(\{p\})}{N} = - \sum_i p_i \log \frac{p_i}{w_i} - \log \omega \doteq \underbrace{\log \rho(\{p\})}_{\text{microcanonical functional}}$$

The Most Probable Distribution is

$$p_i^* = w_i \frac{e^{-\beta x_i}}{q}$$

with

$$\log \omega = \beta \bar{x} + \log q$$

$$\bar{x} = \frac{d \log q}{d \beta}, \quad \beta = \frac{d \log \omega}{d \beta}, \quad \rho(\{p^*\}) = 0.$$



All distributions satisfy

$$\log \omega \geq - \sum_i p_i \log \frac{p_i}{w_i}$$

with the equal sign for $p_i = p_i^*$. This variational condition defines the rank of distributions in the ensemble and identifies the Most Probable Distribution by

$$\log \omega = - \sum_i p_i^* \log$$

Results

$$\rho = - \sum_i p_i \log \frac{p_i}{w_i} - \log \omega$$

$$\rho(\{p\}) \leq 0$$

$$p_i^* = w_i \frac{e^{-\beta x_i}}{q}$$

$$\log \omega = \beta \bar{x} + \log q$$

$$\bar{x} = \frac{d \log q}{d \beta}$$

$$\beta = \frac{d \log \omega}{d \beta}$$



Take x_i to be the energy level of an (N, V) system:

x_i	$\rightarrow$	E
β	$\rightarrow$	$1/kT$
w_i	$\rightarrow$	number of microstates with energy E <i>= thermodynamic entropy</i>
ω	$\rightarrow$	microcanonical partition function
q	$\rightarrow$	canonical partition function
$\rho(\{p\}) \leq 0$	$\rightarrow$	second law

All thermodynamics is recovered

Results

$$\rho = - \sum_i p_i \log \frac{p_i}{w_i} - \log \omega$$

$$\rho(\{p\}) \leq 0$$

$$p_i^* = w_i \frac{e^{-\beta x_i}}{q}$$

$$\log \omega = \beta \bar{x} + \log q$$

$$\bar{x} = \frac{d \log q}{d\beta}$$

$$\beta = \frac{d \log \omega}{d\beta}$$



- *Any* distribution $f(x)$ defined in $(0 \leq x < \infty)$ can be obtained by biased sampling of the exponential distribution using a suitable bias.
- *Any* distribution $f(x)$, $(0 \leq x < \infty)$ satisfies the familiar thermodynamic relationships under a suitable bias.
- *Generalized Thermodynamics* is the probabilistic calculus of the *Most Probable Distribution*. The “ensemble” is the set of all feasible distributions.
- The *Generalized Second Law* states that the Most Probable Distribution is more probable than all other distributions in the feasible space.
- Generalized Thermodynamics applies to probability distributions and by extension to *Stochastic Processes* in general.



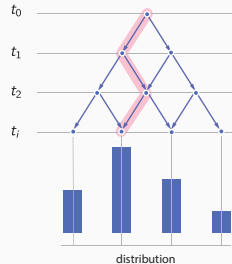
A *stochastic processes* samples distributions of its stochastic variable via *trajectories* in phase space.

A *feasible distribution* is any distribution that can be reached from fixed initial state.

The *microcanonical space* is all distributions that are reached in a fixed number of transitions.

The bias W is fixed by the *transition probabilities* along trajectories.

The *Most Probable Distribution* is the observable *probability distribution* of the stochastic variable.





Evolution is the dynamic transformation of a population clustered by traits, $\mathbf{n} = (n_1, n_2 \dots)$ whose members undergo transitions of the form

$$\alpha'_i X_i + \alpha'_j X_j + \dots \rightarrow \alpha_k X_k + \alpha_l X_l \dots$$

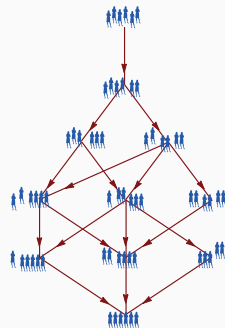
The feasible space is all distributions reached in G steps from fixed initial state. The probability of distribution is

$$P(\mathbf{n}) = \frac{\mathbf{n}! W(\mathbf{n})}{\Omega}$$

with $\mathbf{n} = N! / n_1! n_2! \dots$. The most probable distribution is

$$\frac{n_i^*}{N} = w_i \frac{e^{-\beta i}}{q}$$

The key to unlocking the thermodynamics of the population lies in the *transition probabilities*



Scientific Reports **5** 8855,
2015. <https://doi.org/10.1038/srep08855>



Thermodynamics *is* a universal language: It is the language of probability distributions and stochastic process and we have just began to decipher its grammar

T. Matsoukas, *Generalized Statistical Mechanics*, Springer 2018;

<https://doi.org/10.1007/978-3-030-04149-6>

T. Matsoukas. *Entropy* 2019, 21(9), 890; <https://doi.org/10.3390/e21090890>

