Five axioms are required for a proof of the second law of thermodynamics that uses the Kullback-Leibler divergence.

Brendan Lucas

Consider a physical universe with random, discrete, generalized[1] energy E. The second law follows from these five axioms:

Axiom 1. Energy is a discrete random variable E in a sample space $\mathcal{E} \ni E_i \forall i$ with marginal probability $p(E)$[2].

Axiom 2. The expected energy $\langle E \rangle = \sum_i p_i E_i$ of the universe is a constant.

Axiom 3: If the universe is not in an equilibrium, it will be in equilibrium.

Axiom 4: The set of all energies $\mathcal{E}$ does not change, even as the distribution $p(E)$ may change. In other words, $\mathcal{E}$ is invariant.

Axiom 5: The temperature of the universe is a constant.

You may not be inclined to accept these axioms as a physical reality. Certainly, they are dubious. But they are also inuitive; Axiom 1 mirrors the insights of quantum mechanics, Axiom 2 mirrors what we call the first law of thermodynamics (which we need not assume its traditional form), Axiom 3 almost constitutes the very definition of equilibrium, and Axiom 4 establishes energy as something objective, while the (apparently Bayesian) probabilities can be subjective. Axiom 5, I will not deny, is almost certainly false.

"Proof" of these axioms is out of scope; they may all be false. But we show they are sufficient to prove the second law of thermodynamics, so that is special about them. "Fluctuation theorems" only come so close; they only show an *expectation value* of a change in entropy to be non-negative, not the change in entropy itself.[3]

"Statistical mechanics," as it is commonly understood, we call "the equilibrium theory." This is because "The generalized Boltzmann distribution $p_{\text{eq}}(E_i) = \frac{e^{-E_i/k_B T}}{\sum_j e^{-E_j/k_B T}}$ is the only distribution for which the Gibbs-Shannon entropy $H = -\sum_i p_i \ln p_i$ is equal to the thermodynamic entropy $S = k_B H$. (Gao 2019 [https://arxiv.org/abs/1903.02121])" The generalized Boltzmann distribution *is* the maximum entropy distribution, the equilibrium distribution, so we call it p_{eq}. Away from equilibrium (that is to say, *in real life*), thermodynamic

[1] You may prefer one related to enthalpy, $E_i = \varepsilon_i + pV_i$, or involve a chemical potential like $E_i = \varepsilon_i \pm \mu N_i$, where ε_i is defined so that $\sum_i p_i \varepsilon_i = U$ is the internal energy, or something else. The math works out the same, but the exact expression of the (generalized) free energy will be different. Henceforth "generalized energy" is just "energy."

[2] $p(E)$ describes the frequency at which different values of E can be observed, or assigns a degree of subjective belief to each possible energy level.

[3] "Whither Time's Arrow?" by Gavin E. Crooks

entropy[4] has not been demonstrated to have statistical definition[5]. They won't tell you that in school! But for this derivation, we concern ourselves solely with the Gibbs-Shannon entropy, and do not worry about different thermodynamic entropies or generalized entropies such as those of Tsallis or Renyi.

p_{now} is our model of the universe's energy now, and p_{eq} is the unique marginal of $\mathcal{E}$'s equilibrium; p_{eq} is "the heat death of the universe." $\beta = 1/k_B T$ is inverse temperature, or coldness of the universe. p_{now} is compared against p_{eq} with the Kullback-Leibler divergence (KLD). p_{now} can be any marginal over $\mathcal{E}$, including the equilibrium distribution (but hopefully not, if one likes to live). *The fourth axiom is required to define the KLD.*

1. Define KLD:

$$D[p_{\text{now}} \| p_{\text{eq}}] = \sum_{i=1}^{N} p_{\text{now}}(E_i) \ln\left(\frac{p_{\text{now}}(E_i)}{p_{\text{eq}}(E_i)}\right) = \sum_{i=1}^{N} p_{\text{now}}(E_i) \ln p_{\text{now}}(E_i) - \sum_{i=1}^{N} p_{\text{now}}(E_i) \ln p_{\text{eq}}(E_i)$$

2. Expand and add a special zero

$$\begin{aligned} D[p_{\text{now}} \| p_{\text{eq}}] &= \sum_{i=1}^{N} p_{\text{now}}(E_i) \ln p_{\text{now}}(E_i) - \sum_{i=1}^{N} p_{\text{now}}(E_i) \ln p_{\text{eq}}(E_i) \\ &\quad + \left(\sum_{i=1}^{N} p_{\text{eq}}(E_i) \ln p_{\text{eq}}(E_i) - \sum_{i=1}^{N} p_{\text{eq}}(E_i) \ln p_{\text{eq}}(E_i)\right) \end{aligned}$$

3. Convert to macroscopic variables with $\frac{1}{k_B} S = -\sum_{i=1}^{N} p_i \ln p_i$

$$\begin{aligned} D[p_{\text{now}} \| p_{\text{eq}}] &= \frac{1}{k_B}\Delta S - \sum_{i=1}^{N} p_{\text{now}}(E_i) \ln p_{\text{eq}}(E_i) \\ &\quad + \sum_{i=1}^{N} p_{\text{eq}}(E_i) \ln p_{\text{eq}}(E_i) \\ &= \frac{1}{k_B}\Delta S + \sum_{i=1}^{N} [p_{\text{eq}}(E_i) - p_{\text{now}}(E_i)] \ln p_{\text{eq}}(E_i) \end{aligned}$$

4. Plug in the "heat death" partition function: $p_{\text{eq}}(E_i) = \frac{e^{-\beta E_i}}{\sum_{j=1}^{N} e^{-\beta E_j}} = \frac{e^{-\beta E_i}}{Z}$,

$$\begin{aligned} D[p_{\text{now}} \| p_{\text{eq}}] &= \frac{1}{k_B}\Delta S + \sum_{i=1}^{N} [p_{\text{eq}}(E_i) - p_{\text{now}}(E_i)] \ln\left(\frac{e^{-\beta E_i}}{\sum_{j=1}^{N} e^{-\beta E_j}}\right) \\ &= \frac{1}{k_B}\Delta S + \sum_{i=1}^{N} [p_{\text{now}}(E_i) - p_{\text{eq}}(E_i)] \cdot [\beta E_i] + \sum_{i=1}^{N} [p_{\text{now}}(E_i) - p_{\text{eq}}(E_i)] \ln Z \end{aligned}$$

[4] "Thermodynamic entropy" is entropy as it was understood by Clausius and Kelvin, or now by chemists and some (e.g. mechanical) engineers.

[5] "Gibbs-Shannon entropy" is the definition preferred by many theorists and other (e.g. electrical) engineers.

5. Notice that

$$\sum_{i=1}^{N}[p_{\text{now}}(E_i) - p_{\text{eq}}(E_i)] \ln Z = \ln Z[\sum_{i=1}^{N} p_{\text{now}}(E_i) - \sum_{i=1}^{N} p_{\text{eq}}(E_i)] = \ln Z - \ln Z = 0$$

   So,

$$D[p_{\text{now}} \| p_{\text{eq}}] = \frac{1}{k_B}\Delta S + \sum_{i=1}^{N}[p_{\text{now}}(E_i) - p_{\text{eq}}(E_i)] \cdot [\beta E_i]$$

6. The following step gives a difference in the expectation values of energy if and only if every E_i is the same in p_{eq} and p_{now}; axiomatically, the energy levels did not change, but only their probabilities changed.

$$\begin{aligned} D[p_{\text{now}} \| p_{\text{eq}}] &= \frac{1}{k_B}\Delta S + \sum_{i=1}^{N} p_{\text{now}}(E_i)\beta E_i - \sum_{i=1}^{N} p_{\text{eq}}(E_i)\beta E_i \\ &= \frac{1}{k_B}\Delta S - \beta\Delta\langle E\rangle \end{aligned}$$

7. Invoke the second axiom,

$$k_B D[p_{\text{now}} \| p_{\text{eq}}] = \Delta S,$$

8. KLD is non-negative, so

$$\Delta S \geq 0$$

QED, that is the second law of thermodynamics, in all the glory of its shaky foundation. **The entropy of a universe with these five axioms can only increase or stay the same, but never decrease!**