Entropy for Data Science

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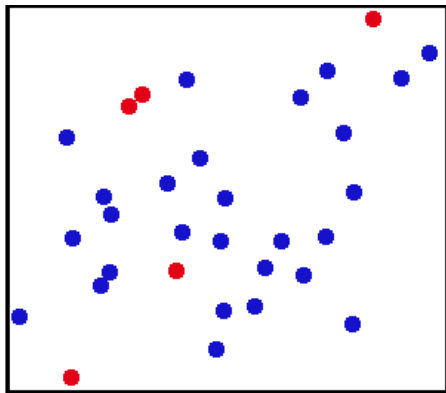
Outline

- History
  - Statistical Mechanics
- Shannon Entropy
  - Uniform Distribution
  - Normal Distribution
  - Tsallis Entropy
- Entropy for Data Science

History

Statistical Mechanics

Consider a box with N particles of a monatomic gas

How would you model this?

Statistical Mechanics - State Variables?

- We can talk about state variables: P, T, N, and V

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$$PV = nRT \tag{1}$$
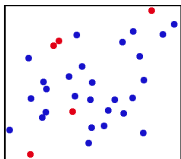
Statistical Mechanics - State Variables?

- We can talk about state variables: P, T, N, and V
  - Ideal Gas Law

$$PV = nRT \tag{1}$$

- Characterize System Behaviors
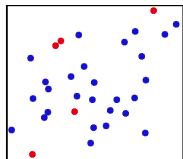
Statistical Mechanics - Ensemble Statistics

Assume each particle obeys Newton's Law

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James Maxwell's Kinetic Theory of Gases

- Consider Ensemble Statistics

$$PV = \frac{Nm\bar{v^2}}{3} \qquad (2)$$

Statistical Mechanics Entropy

Average Behavior $\rightarrow$ Macroscopic Properties

Statistical Mechanics Entropy

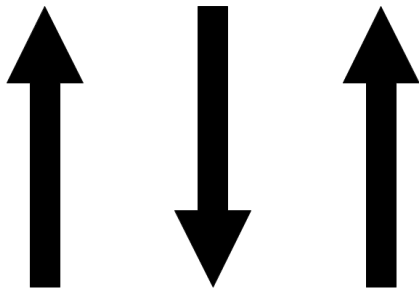Average Behavior $\rightarrow$ Macroscopic Properties

Ludwig Boltzmann's statistical mechanical entropy (1877)

$$S = k_b \ln(\Omega) \tag{3}$$

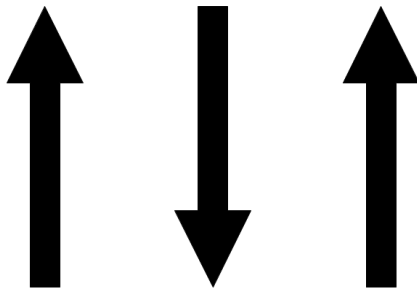Ω is the multiplicity of a given macrostate

Macrostates, Microstates, and Multiplicity

Consider non-interacting paramagnet with 3 dipoles

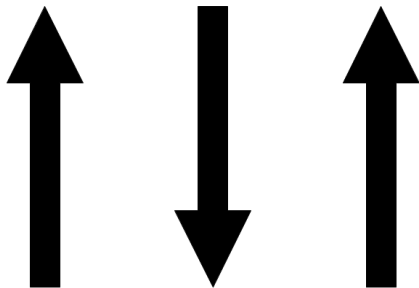## Macrostates, Microstates, and Multiplicity

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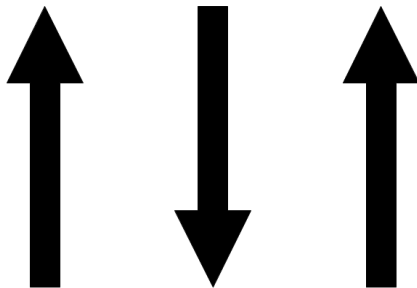
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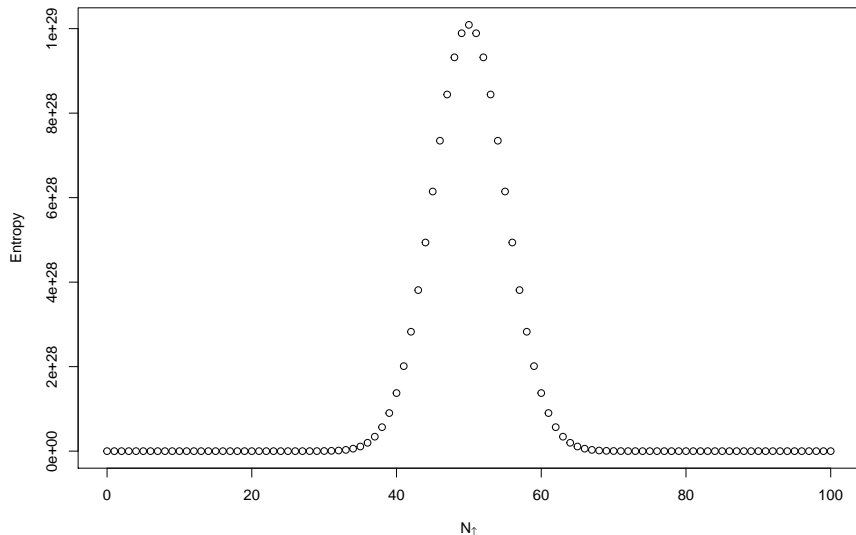

- Macrostate - 2 Up, 1 Down
- Microstate - ↑, ↓, ↑

Macrostates, Microstates, and Multiplicity

Consider non-interacting paramagnet with 3 dipoles

- Macrostate - 2 Up, 1 Down
- Microstate - $\uparrow$, $\downarrow$, $\uparrow$
- $\Omega = \binom{N}{N_\uparrow} = \binom{3}{2}$

Entropy of 100 Dipole Paramagnet

Interpretation

Features of paramagnet entropy

- Minimum at 0 and $100 \rightarrow 1$ microstate each
- Maximum at $50 \rightarrow 10^{29}$ microstates!

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Measure of "mixed-up-ness" of a physical system

- Higher entropy $\rightarrow$ more mixing (randomness)
- Lower entropy $\rightarrow$ less mixing

Shannon Entropy

Telephone Line Information Loss

Claude Shannon at Bell Telephone (1939)

- Quantify "lost information" in phone-line signals
- "Information Uncertainty"

$$H = -K \sum_{i=1}^{k} p(i) \log(p(i)) \tag{4}$$

Difficult time naming H...

Naming "Information Uncertainty"

. . . until he visited John von Neumann

My greatest concern was what to call it. I thought of calling it 'information', but the word was overly used, so I decided to call it 'uncertainty'. When I discussed it with John von Neumann, he had a better idea. Von Neumann told me, 'You should call it entropy, for two reasons: In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, nobody knows what entropy really is, so in a debate you will always have the advantage.

Shannon Entropy

Same properties as statistical mechanic entropy

- Low entropy $\rightarrow$ low randomness
- High entropy $\rightarrow$ high randomness

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- Average information content

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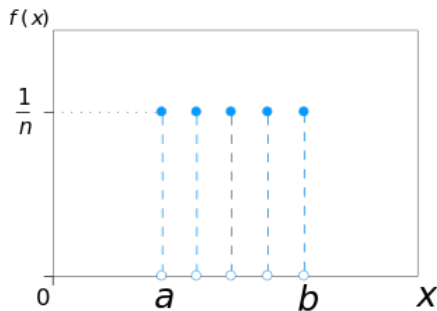- High entropy $\rightarrow$ high randomness

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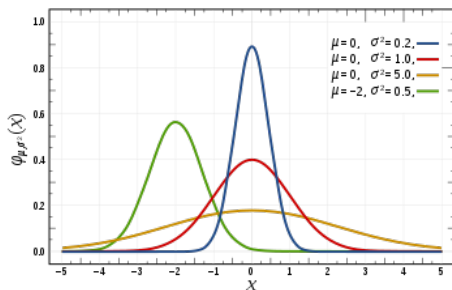- Average information content

$$H(X) = E[-\ln(X)] \tag{5}$$

Shannon Entropy - Uniform Distribution

- Maximum Entropy
  - $H(X) = \ln(N)$
- Boltzmann Statistical Mechanics Entropy
  - $S = k_b \ln(\Omega)$

Shannon Entropy - Normal Distribution

- Maximum Entropy for fixed mean and variance
  - $H(X) = \frac{1}{2} \log(2\pi e \sigma^2)$
- Part of the reason *why the normal distribution*

Tsallis Entropy

Attempt to generalize statistical mechanics

$$S_q(p_i) = \frac{k}{q-1}\left(1 - \sum_i p_i^q\right) \tag{6}$$

- q is entropic-index
  - $q \to 1$, recover Shannon Entropy
- Experimental Verification
  - Physical significant still debated

Entropy for Data Science

Anamoly Detection

- Entropy for detecting changes in "randomness"
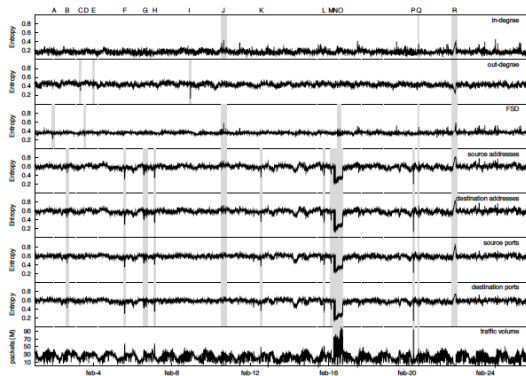 - ▶ Machine Learning and Metric Entropy

Figure 1: Nychis et. al. 2008

Anamoly Detection - Tsallis Entropy

- Similar work with Tsallis Entropy
  - q values for specific anamolies

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Currently in the works with Akamai!

Summary

- Entropy from Statistical Mechanics
  - Measure of "mixedness" or macrostate
- Adopted by Shannon $\rightarrow$ Infromation Loss
  - Average Information of State
  - Unpredictability
- Applicaitons in Anamoly Detection