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Course 565/665 Lecture Number ______ Date 2/20/03

Lecturer Dr. Silvia Cavagnero Note Taker Eric Fulmer

Last Time

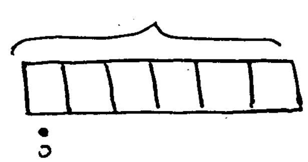
We used the maximum S principle to derive

$$\frac{p_i^*}{\sum_{i=1}^{t} p_i^*} = \frac{1}{t} \quad \Leftarrow \text{ Flat distribution}$$

in the absence of constraints (with the exception that the p_i's are normalized).
t is the number of outcomes.

In real life, we typically gain knowledge about averages. Since we know the average of the quantity, we can use this as a constraint. [Implicit assumptions: events have an associate score.]

$\varepsilon_i \equiv$ individual score per event.



$\leftarrow N$

t

N = # of 1D lattice points (boxes).

$$E = \sum_{i=1}^{t} \varepsilon_i n_i$$

↑ total score

n_i is the number of outcomes of a particular energy level (of a particular ε_i score).

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Q: Expected Distribution that satisfies the following

$$\langle \varepsilon \rangle = \frac{E}{N} = \frac{1}{N}\sum_{i=1}^{t} n_i \varepsilon_i = \sum_{i=1}^{t} \frac{n_i}{N}\varepsilon_i = \sum_{i=1}^{t} p_i \varepsilon_i$$

AND it satisfies the S_{MAX} principle?

ie, what is $\{p_1^*, p_2^*, \ldots, p_t^*\}$ that maximizes S?

$$g(p_1, p_2, \ldots p_t) = \sum_{i=1}^{t} p_i = 1$$

$$\Rightarrow \quad ① \quad \boxed{\sum_{i=1}^{t} dp_i = 0}$$

$$h(p_1, p_2, \ldots p_t) = \langle \varepsilon \rangle = \sum_{i=1}^{t} p_i \varepsilon_i$$

$$\Rightarrow \quad ② \quad \boxed{\sum_{i=1}^{t} \varepsilon_i \, dp_i = 0}$$

Also, we want $\boxed{dS = 0}$ (3)

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Thus, we set up our equation:

$$\left(\frac{\partial S}{\partial p_i}\right) \text{ minus } (\text{A Lagrange Multiplier})\left(\frac{d\,(\text{constraint})}{d\,p_i}\right) = 0$$

to find the set of p_i's that maximizes S.

$$\boxed{\underbrace{\left(\frac{\partial S}{\partial p_i}\right)}_{A} - \alpha \underbrace{\left(\frac{\partial g}{\partial p_i}\right)}_{B} - \beta \underbrace{\left(\frac{\partial h}{\partial p_i}\right)}_{C} = 0}$$

Key Equation to set up.

$$\frac{S}{k} = -\sum p_i \ln p_i$$

let $k = 1$ in this problem.

$\underline{A} = -\ln p_i - 1$

$\underline{B} = 1$

$\underline{C} = \varepsilon_i$

Rewrite the Key Equation from above:

$$\boxed{-\ln p_i - 1 - \alpha - \beta \varepsilon_i = 0}$$

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We would like to solve for the pi that satisfies the three constraints and thus maximizes the S (entropy) with respect to that probability. Let this pi be p_i^*.

$$-1 - \ln p_i^* - \alpha - \beta \varepsilon_i = 0$$

$$\ln p_i^* = -1 - \alpha - \beta \varepsilon_i$$

$$p_i^* = e^{-1-\alpha-\beta\varepsilon_i} = e^{-1-\alpha} e^{-\beta\varepsilon_i}$$

Normalizing pi,

$$p_i^* = \frac{p_i^*}{\sum_{i=1}^{t} p_i^*} = \frac{\cancel{e^{-1-\alpha}} e^{-\beta\varepsilon_i}}{\sum_{i=1}^{t} \cancel{e^{-1-\alpha}} e^{-\beta\varepsilon_i}}$$

Thus, $$p_i^* = \frac{e^{-\beta\varepsilon_i}}{\sum_{i=1}^{t} e^{-\beta\varepsilon_i}} = \frac{e^{-\beta\varepsilon_i}}{Q}$$ [Boltzmann Distribution]

Where $Q = \sum_{i=1}^{t} e^{-\beta\varepsilon_i}$ [The Partition Function]

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The partition function is an enigmatic quantity, but its essence is much much less ellusive that it would seem. Q [partition function] is only a <u>Normalization Factor</u> for the $e^{-\beta\varepsilon_i}$ statistical weight. It is only the sum of all of the statistical weights, and it ensures that the sum of all of the p_i's equals one. Remember, Q is only a constant, and it normalizes the weights. But the power of Q will be demonstrated later, as important quantities can be extracted from it (such as the free energy, etc).

$$p_i^* = \frac{e^{-\beta\varepsilon_i}}{\sum_{i=1}^{\infty} e^{-\beta\varepsilon_i}}$$

$$\boxed{\begin{aligned}\langle\varepsilon\rangle &= \sum_{i=1}^{\infty} p_i^* \varepsilon_i \\ &= \frac{1}{Q}\sum_{i=1}^{\infty} \varepsilon_i e^{-\beta\varepsilon_i}\end{aligned}}$$

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Example | Rolling a Die.

1) $t=6$ (faces of a die)

2) $\varepsilon_i \equiv i$ [possible scores $i = \{1,2,3,4,5,6\}$

3) $e^{-\beta} \equiv x$

Thus, $e^{-\beta\varepsilon_i} = (e^{-\beta})^{\varepsilon_i} = x^{\varepsilon_i} = x^i$ [from above]

Defining the Partition Function:

$$Q = \sum_{i=1}^{6} e^{-\beta\varepsilon_i} = \sum_{i=1}^{6} x^i = x + x^2 + x^3 + x^4 + x^5 + x^6$$

$$p_i^* = \frac{x^i}{\sum_{i=1}^{6} x^i} = \frac{x^i}{x + x^2 + x^3 + x^4 + x^5 + x^6}$$

$$\langle\varepsilon\rangle = \sum_{i=1}^{6} \varepsilon_i p_i^* = \sum_{i=1}^{6} i\, p_i^* = \frac{x + 2x^2 + 3x^3 + 4x^4 + 5x^5 + 6x^6}{x + x^2 + x^3 + x^4 + x^5 + x^6}$$

Remember, $\langle\varepsilon\rangle$ is only a number.

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If $e^{-\beta} = x = 1$, then there is not a weighting factor depending on the state of the system (or the energy level). Each state would be equally likely.

$$\langle \varepsilon \rangle = \frac{1+2+3+4+5+6}{1+1+1+1+1+1} = 3.5$$

We know this because

$$\langle \varepsilon \rangle = 3.5 = \frac{x+2x^2+3x^3+4x^4+5x^5+6x^6}{x+x^2+x^3+x^4+x^5+x^6}$$

Solving, $x = 1$.

$$p_i^* = \frac{1}{6} = \frac{1}{t}$$ flat distribution.

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If the average were weighted differently,

$\langle \varepsilon \rangle = 3.0$ biased

Solve for x,

$x = 0.84$ $(\neq 1)$

$p_i = 0.25, 0.21, 0.17, \ldots$