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Course 565/665 Lecture Number ______ Date 2/14/03

Lecturer Dr. Silvia Cavagnero Note Taker Eric Fulmer

Method of Undetermined LaGrange Multipliers

- This method is absolutely necessary for the development of Statistical Mechanics (Just for your information).

Multivariate functions w/ constraints

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy = 0 \qquad (1)$$

$$dg = \left(\frac{\partial g}{\partial x}\right)_y dx + \left(\frac{\partial g}{\partial y}\right)_x dy = 0 \qquad (2)$$

From (1), $\frac{dy}{dx} = -\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial y}{\partial f}\right)_x$

From (2), $\frac{dy}{dx} = -\left(\frac{\partial g}{\partial x}\right)_y \left(\frac{\partial y}{\partial g}\right)_x$

The df above is equal to ~~an ext~~ zero because we seek to find an extremum of the function $f(x,y)$.

The dg above is equal to zero because it is a constraint, thus equaling a constant.

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From before,

$$\frac{dy}{dx} = \frac{(\partial f/\partial x)_y}{(\partial f/\partial y)_x} = \frac{(\partial g/\partial x)_y}{(\partial g/\partial y)_x} \qquad (3)$$

$$\left(\frac{\partial f}{\partial x}\right)_y = \lambda \left(\frac{\partial g}{\partial x}\right)_y$$

$$\left(\frac{\partial f}{\partial y}\right)_x = \lambda \left(\frac{\partial g}{\partial y}\right)_x$$

The above 2 equations are true because relation (3) requires the equality of 2 rations, implying that the derivatives of f and g need only to be the same within an arbitrary constant λ (the Lagrange Multiplier).

$$\left(\frac{\partial f}{\partial x}\right)_y - \lambda \left(\frac{\partial g}{\partial x}\right)_y = 0$$

$$\left(\frac{\partial f}{\partial x}\right)_x - \lambda \left(\frac{\partial g}{\partial x}\right)_y = 0$$

We also have the original constraint $g(x,y) = 0$.

Thus, we have 3 equations for 3 unknowns,

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By solving the above 3 equation, we can solve for x^* and y^*, which give us the extremum of $f(x,y)$ taking into account the $g(x,y)$.

For a more general case:

$x_1, x_2, \ldots, x_t$ (independent variables)

$g(x_1, \ldots), h(x_1, \ldots)$ (constraints)

Using the same development from pages 1 and 2,

$$\frac{\partial f}{\partial x_1} - \lambda \frac{\partial g}{\partial x_1} - \beta \frac{\partial h}{\partial x_1} + \ldots = 0$$

$$\ldots \quad \ldots \quad \ldots \quad \ldots = 0$$

$$\frac{\partial f}{\partial x_t} - \lambda \frac{\partial g}{\partial x_t} - \beta \frac{\partial h}{\partial x_t} - \ldots = 0$$

$\lambda, \beta, \ldots$ are the Lagrange Multipliers.

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$$df = \sum_{i=1}^{t} \left(\frac{\partial f}{\partial x_i}\right)_{j \neq i} dx_i = 0$$

$$dg = \sum_{i=1}^{t} \left(\frac{\partial g}{\partial x_i}\right)_{j \neq i} dx_i$$

In General:

$$\sum_{i=1}^{t} \left[\left(\frac{\partial f}{\partial x_i}\right)_{j \neq i} dx_i - \lambda \left(\frac{\partial g}{\partial x_i}\right)_{j \neq i} dx_i - \beta \left(\frac{\partial h}{\partial x_i}\right)_{j \neq i} dx_i - \cdots \right] = 0$$

$$\sum_{i=1}^{t} \left[\left(\frac{\partial f}{\partial x_i}\right)_{j \neq i} - \lambda \left(\frac{\partial g}{\partial x_i}\right)_{j \neq i} dx_i - \beta \left(\frac{\partial h}{\partial x_i}\right)_{j \neq i} dx_i \cdots \right] dx_i = 0$$

Example 5.6 Parabola in 3D.

$$x^2 + y^2 = f(x,y)$$
$$x + y = 6 = g(x,y)$$
$$x + y - 6 = 0 = g(x,y)$$

$$\left(\frac{\partial f}{\partial x}\right)_y = 2x \qquad \left(\frac{\partial f}{\partial y}\right)_x = 2y$$

$$\left(\frac{\partial g}{\partial x}\right)_y = 1 \qquad \left(\frac{\partial g}{\partial y}\right)_x = 1$$

$$\left(\frac{\partial f}{\partial x}\right)_y - \lambda \left(\frac{\partial g}{\partial x}\right)_y = 0 \qquad \left(\frac{\partial g}{\partial y}\right)_x - \lambda \left(\frac{\partial g}{\partial y}\right)_x = 0$$

$$2x - \lambda = 0 \qquad 2y - \lambda = 0$$

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Thus, our 3 equations are

$$2x - \lambda = 0$$
$$2y - \lambda = 0$$
$$x + y - 6 = 0$$

$$\lambda = 2x$$
$$2y - 2x = 0$$
$$2y = 2x$$
$$y = x$$

$$x + y = 6$$
$$x + x = 6$$

$$\boxed{\begin{array}{c} x = 3 \\ y = 3 \\ \lambda = 6. \end{array}}$$

$f(3,3) = f(x^*, y^*)$ is the extremum of $f(x,y)$ subject to the constraint $g(x,y) = x + y = 6$.

Chapter 6

Entropy + The Boltzmann Law

$$S = k_B \ln W$$

S is the entropy

k_B (or k) is the Boltzmann Constant

$$k_B = 1.380662 \times 10^{-23} \text{ J K}^{-1} \quad [\text{Energy}/\text{Temperature}]$$

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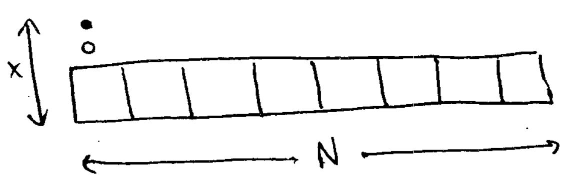
This is a very <u>profound equation.</u> The macroscopic quantity Entropy (S) is proportional to the natural logrithm of the Multiplicity of the System (W). The proportionality constant of this relation is k_B, the Boltzmann Constant, and this is a <u>Universal Constant</u> found in many other equation that describe our reality.

<u>Probability Formulation of S</u>

Stirling's Approximation: $\ln n! = n\ln n - n$

$$n! \approx \left(\frac{n}{e}\right)^n$$ ← [See the Book — Chapter 4]

Given 

$$W = \frac{N!}{n_1!\, n_2! \cdots n_t!}$$ where $N = n_1 + n_2 + \cdots + n_t$

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$p_i = \frac{n_i}{N}$ From Stirling's: $n! \approx \left(\frac{n}{e}\right)^n$

$$W = \frac{\left(\frac{N}{e}\right)^N}{\left(\frac{n_1}{e}\right)^{n_1}\left(\frac{n_2}{e}\right)^{n_2}\cdots\left(\frac{n_t}{e}\right)^{n_t}} = \frac{e^{N} \quad N^N}{e^{n_1+n_2+\cdots+n_i} \cdot n_1^{n_1} n_2^{n_2}\cdots n_t^{n_t}}$$

$$= \frac{N^{(n_1+n_2+n_3+\cdots+n_t)}}{n_1^{n_1} n_2^{n_2}\cdots n_t^{n_t}} = \frac{N^{n_1} N^{n_2}\cdots N^{n_t}}{n_1^{n_1} n_2^{n_2}\cdots n_t^{n_t}}$$

$$= \left(\frac{N}{n_1}\right)^{n_1}\left(\frac{N}{n_2}\right)^{n_2}\cdots\left(\frac{N}{n_t}\right)^{n_t} = \frac{1}{p_1^{n_1} p_2^{n_2}\cdots p_t^{n_t}}$$

$$W = \frac{1}{p_1^{n_1} p_2^{n_2}\cdots p_t^{n_t}}$$

$$\frac{\ln W}{N} = -\frac{1}{N}\sum_{i=1}^{t} n_i \ln p_i = -\sum_{i=1}^{t} p_i \ln p_i$$

$$\frac{S}{kN} = -\sum_{i=1}^{t} p_i \ln p_i$$

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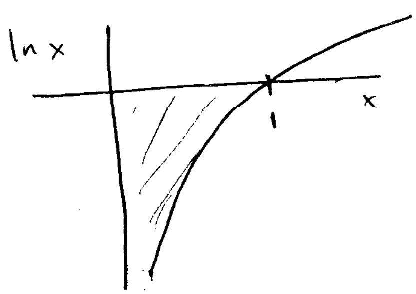
Thus, $\frac{S_N}{k} = -\sum_{i=1}^{t} p_i \ln p_i$ where $S_N = \frac{S}{N}$

p_i is the probability of a given event/outcome.



If $p_i = 1$, then the $\ln p_i = 0$.

If only one outcome is possible, then entropy is zero (very small).