Stationary states of opinion diffusion

Project for the exam: AMS (DSE)

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Theoretical Framework

Statistical Mechanics

"Ludwig Boltzmann, who spent much of his life studying statistical mechanics, died in 1906, by his own hand. Paul Ehrenfest, carrying on the work, died similarly in 1933. Now it is our turn to study statistical mechanics." States of Matter (1975), by David L. Goodstein

Concepts of statistical mechanics: entropy [1]

Central problem of thermodynamics: characterize the actual state of equilibrium among all virtual states

Entropy postulate: there exist a function S of the extensive variables $(X_0, X_1 ... X_r)$ called entropy, that assumes the maximum value for a state of equilibrium among all vritual states and that possesses the following properties:

- Extensivity $S^{(1 \cup 2)} = S^1 + S^2$
- Convexity $S((1-\alpha)X^1 + \alpha X^2) \geq (1-\alpha)S(x^1) + \alpha S(X^2)$
- Monotonicity $\frac{\partial S}{\partial E}|_{X_1 ... X_r} = \frac{1}{T} > 0$

The equilibrium state corresponds to the maximum entropy compatible with the constrains

Concepts of statistical mechanics: entropy [1]

- **Fundamental postulate of statistical mechanics**
  $S = k_b \ln |\Gamma|$
- Where S is the thermodynamic entropy, k_b is Boltzmann constant and $|\Gamma|$ the volume in the phase space

$$S(X_0, ..., X_r) = k_b \ln \int_\Gamma dx = k_b \int dx \prod_{i=0}^{r} [\theta(X_i(x) - (X_i - \Delta X_i))\theta(X_i - X_i(x))] \quad (1)$$

- $(X_0, ..., X_r)$ are the extensive variables
- The θ functions assures that the integrand is not null only in the interval $X_i - \Delta X_i \leq X_i(x) \leq X_i$

Concepts of statistical mechanics: micro-canonical ensamble

- Lets focus on a particular observable A (extensive)

$$S(X;a) = k_b \ln \int_\Gamma dx \delta(A(x) - a) \tag{2}$$

$$S(X) = S(X;a*) \geq S(X;a) \tag{3}$$

$$\begin{aligned} \frac{|\Gamma(a)|}{|\Gamma|} &= \frac{1}{|\Gamma|} \int_\Gamma dx \delta(A(x) - a)) \\ &= \exp\left\{ \frac{1}{k_b} \left[S(X;a) - S(X;a^*) \right] \right\} \\ &\simeq \exp\left\{ \frac{1}{k_b} \left[\frac{\partial^2 S}{\partial A^2} |_{a^*} (a - a^*)^2 \right] \right\} \end{aligned} \tag{4}$$

$$a^* = \langle A(x) \rangle = \frac{1}{|\Gamma|} \int_\Gamma dx A(x) \tag{5}$$

Concepts of statistical mechanics: canonical ensemble

$$a^* = \frac{1}{|\Gamma|} \int_\Gamma dx_s dx_R A(x_s) \tag{6}$$

$$\langle A(x) \rangle = \int dx_s dx_r A(x_S) \delta(H^{(s)} \tag{7}$$

$$\langle A(x) \rangle = \frac{1}{|\Gamma|} \int dx_s dx_r A(x_s) \delta(H^S(x_s) + H^R(x_R) - H^S(x_S)) \tag{8}$$

$$\langle A(x) \rangle = \frac{1}{|\Gamma|} \int dx_s A(x_s) \times \int dx_r \delta(H^R(x_R) - (E - H^{(S)}(x_s))) \tag{9}$$

$$\int dx_r \delta(H^R(x_R) - (E - H^{(S)}(x_s))) \simeq \exp\left\{ \frac{1}{k_b} S^R(E - H^S) \right\} \tag{10}$$

Concepts of statistical mechanics: canonical ensemble

$$\exp\left\{\frac{1}{k_b}S^R(E-H^S)\right\} \simeq \exp\left[\frac{1}{k_b}S^R(E)\right]\exp\left[-\frac{1}{k_b}\frac{\partial S^{(R)}}{\partial E}|_E H^{(S)}(x_S)\right] \tag{11}$$

$$\langle A(x)\rangle = \frac{1}{Z}\int dx_s A(x_s) exp\left[-\frac{H^{(S)}(x_s)}{k_b T}\right] \tag{12}$$

$$Z = \int dx_s exp\left[-\frac{H^S(x_s)}{k_b T}\right] \tag{13}$$

$$\langle A(x)\rangle = \frac{1}{Z}\int dE \int dx \delta(H(x)-E) A(x) exp(-\frac{E}{k_b T}) \tag{14}$$

$$\langle A(x)\rangle = \frac{1}{Z}\int dE' a^*(E') exp\left[-\frac{E'-TS(E')}{k_b T}\right] \tag{15}$$

Concepts of statistical mechanics: canonical ensemble[1]

$$Z \simeq \exp\left[-\frac{E* - TS(E*)}{k_b T}\right] = \exp\left(-\frac{F}{k_b T}\right) \quad (16)$$

$$\frac{\partial lnZ(\beta)}{\partial \beta} = -\frac{1}{Z}\int dx H(x) \exp\left[-\frac{H}{k_b T}\right] = -\langle H(x)\rangle = -E \quad (17)$$

$$\frac{\partial^2 lnZ(\beta)}{\partial \beta^2} = \left\langle H(x)^2 \right\rangle - \langle H(x)\rangle^2 \quad (18)$$

$$\left\langle H(x)^2 \right\rangle - \langle H(x)\rangle^2 = -\frac{\partial E}{\partial(1/k_b T)} = k_b T^2 \frac{\partial E}{\partial T} = k_b T^2 C \quad (19)$$

In this way a statistical quantity the variance has been connected to a thermodynamic quantity: the temperature.

Numerical simulations

"Never make a calculation until you know the answer. Make an estimate before every calculation, try a simple physical argument (symmetry! invariance! conservation!) before every derivation, guess the answer to every paradox and puzzle. Courage: No one else needs to know what the guess is. Therefore make it quickly, by instinct. A right guess reinforces this instinct. A wrong guess brings the refreshment of surprise. In either case life as a spacetime expert, however long, is more fun!" John Archibald Wheeler

Numerical simulation [1]

- **Simulation** *the evolution equations of a system are defined to such a detail that a computer can make its behaviour explicit, and one looks to see what takes place*
- Numerical experiment
- **Molecular dynamics:** the equation of motion are solved numerically PROS: information of both the dynamical and static properties of the system are explored
- **Monte Carlo:** a fictitious evolution process of the system is solved in order to get the equilibrium distribution PROS 1) also the systems whose dynamics is not defined can be explored 2) a fictitious dynamics can be considered in order to reach the equilibrium faster
- Molecular dynamics may provide a proof of statistical mechanics, Monte Carlo methods presuppose its validity

Monte Carlo method [1]

- We would calculate an integral of type $\langle A \rangle = \int dx A(x) \rho(x)$ where ρ is the probability distribution.
- Evaluate the integrand in N+1 points uniformly arranged between 0 and 1 $\langle A \rangle = \frac{1}{N} \sum_{i=0}^{N} A(x_i) \rho(x_i)$
- A better convergence is reached if the x_i density is proportional to $\rho(x)$

Monte Carlo method [1]

- The quantity $\langle A \rangle$ is evaluated over a distribution $\rho(x)$ where x_i are random, independent and distributed with a probability density $\rho(x)$
- The independence conditions can be relaxed with the condition that the correlations between $x_i and x_{i+l}$ go to zero fairly rapidly as l grows
- The true dynamics is replaced with a fictitious stochastic dynamics. The state at $t+1$ depends only from the state at t. $\rightarrow$ Markov Chain

Monte Carlo method [1]

- The evolution of probability is described by the **master equation** $\Delta p_a(t) = \sum'_{b\neq a}[W_{ab}p_b(t) - W_{ba}p_a(t)]$
- stationary $\rightarrow \sum'_{b\neq a}[W_{ab}p_b(t) - W_{ba}p_a(t) = 0 \quad \forall a$
- Detailed balance property $W_{ab}W_{bc}W_{ca} = W_{ac}W_{cb}W_{ba}$
- $W_{ab}p_b(t) - W_{ba}p_a(t) = 0 \quad \forall a, b$

Monte Carlo method [1]

- We would sample p_a^{eq}
- This can be performed as long as the W_{ab} is ergodic and the detailed balance property holds
- The transition between any two arbitrary states can take place as long as one waits for a sufficient amount of time

Application [1]

- $H(\sigma) = -\sum_{\langle ij \rangle} J\sigma_i\sigma_j - \sum_i h\sigma_i$
- $P_\sigma = \frac{e^{-H(\sigma)/k_bT}}{Z} \quad Z = \sum_\sigma e^{-H(\sigma)/k_bT}$
- The observable are calculated as
  $E = \langle H \rangle = \sum_{sigma} H(\sigma) P^B_{\sigma'} \quad M = \sum_\sigma (\sigma_i\sigma)\, P^B_\sigma$
- The markov chain states should be the microstates σ and P_σ the stationary distribution
- $W_{\sigma\sigma'} = W_{\sigma'\sigma}\,\dfrac{P_\sigma}{P_{\sigma'}} = W_{\sigma'\sigma}\exp -\dfrac{H(\sigma) - H(\sigma')}{k_bT}$
- The Z term is no more present !!!

Bibliography I

Luca Peliti. *Statistical mechanics in a nutshell*. Princeton University Press, 2011.

ROC and ϕ factor