Maximum Entropy and Maximum Entropy Production

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Introduction

- Problem: We want to predict the *macroscopic* behaviour of a system with many interacting degrees of freedom. For example: Ecosystems, plants, climate, economies...

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- Problem: We want to predict the *macroscopic* behaviour of a system with many interacting degrees of freedom. For example: Ecosystems, plants, climate, economies...
- Traditional solutions: Try to simulate everything in the system. Global circulation models, dynamic ecosystem models
- But statistical physics deals with these kinds of systems all the time. Why not use statistical methods?

Maximum Entropy

The maximum entropy method (Gibbs): Find the probability distribution of microstates i (microscopic arrangements of a system) that maximises the entropy

$$H = -\sum_i p_i \log p_i,$$

subject to the constraints C.

Maximum Entropy

Information theory interpretation (Jaynes):

Behaviour that is experimentally reproducible under conditions C must be theoretically predictable from C alone. We maximise the information entropy of the system subject to the conditions C. A smaller entropy would mean we have added more information that just C.

Maximum Entropy

Example 1: Closed, isolated system in equilibrium

- Number of particles N and total energy E fixed.
- Let probability of microstate (that is, energies of all individual particles, satisfying total energy and the internal physics) i be p_i.
- Let the total number of microstates be $\Omega(N, E)$.

We need to maximise $H = -\Sigma_{i=1}^{\Omega(N,E)} p_i \log p_i$ subject to the constraint $\Sigma_{i=1}^{\Omega(N,E)} p_i = 1$. Use the method of Lagrange multipliers. We seek the maximum of

$$\Phi = -\Sigma_{i=1}^{\Omega(N,E)} p_i \log p_i - \alpha \left(\Sigma_{i=1}^{\Omega(N,E)} p_i - 1 \right)$$

over all possible p_i. Set $d\Phi/dp_i = 0$ and end up with

$$p_i = \frac{1}{\Omega(N, E)}.$$

(Substitute back in and get the Boltzmann entropy $\propto \log \Omega$.)

Maximum Entropy

Example 2: Closed system in equilibrium

- Number of particles N and *average* energy $\bar{E}$ fixed.
- We need to maximise $H = -\Sigma_{i=1}^{\Omega(N,E)} p_i \log p_i$ subject to the constraints $\Sigma_{i=1}^{\Omega(N,E)} p_i = 1$ and $\Sigma_{i=1}^{\Omega(N,E)} p_i E_i = \bar{E}$.

End up with

$$p_i = \frac{1}{Z} \exp(-\beta E_i)$$

More generally, we seek to maximise the *relative* entropy

$$H(p||q) = -\sum_i p_i \log \frac{p_i}{q_i},$$

that is, we minimise the information gained about i by applying the constraints C on the prior q_i. If we were gaining more information, we would be specifying more than the constraints. The prior q_i is the distribution describing *total ignorance* about i.

Maximum Entropy

Application to ecological communities

For species j, let

- r_j denote its per capita resource use [known]
- n_j denote its population.

Here a microstate i is a particular distribution of populations $(n_1, \ldots, n_S)$.
We seek to find the distribution of microstates leading to maximum entropy subject to the constraints:

- Resource use is limited: $\bar{R} = \sum_{j=1}^{S} \bar{n}_j r_j$
- Number of organisms is (initially) limited: $\bar{N} = \sum_{j=1}^{S} \bar{n}_j$.

We make no assumptions about underlying population dynamics (birth, death, dispersal), and we can allow different levels of resource use.

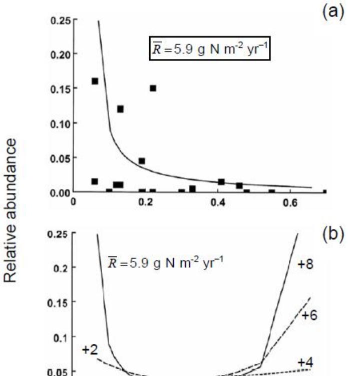
Maximum Entropy

Application to ecological communities

Can derive

- Probability of a microstate i, p_i
- Mean abundance of species j, $\bar{n}_j$
- Mean number of species with abundance n, $s(n)$.

Given the resource use level for each species, can compute all these things.



Maximum Entropy Production

What about non-equilibrium systems? Apply MaxEnt to the microscopic *paths* of the system.
Path entropy: $H(p) = -\sum_\Gamma p_\Gamma \log p_\Gamma$. We seek to maximise this with respect to:

- Normalisation: $\sum_\Gamma p_\Gamma = 1$
- External fluxes $F = \sum_\Gamma p_\Gamma f_\Gamma$ which we know to exist in the system.

Optimising H for the external fluxes H turns out to be equivalent to maximising the system's irreversibility

$$I(p) = \sum_\Gamma p_\Gamma \log \frac{p_\Gamma}{\tilde{p}_\Gamma},$$

in other words the relative entropy of forward paths Γ relative to backward paths $\tilde{\Gamma}$.

Maximum Entropy Production

Applications

Can be used for such things as:

- Horizontal heat flows in Mars, Earth and Titan
- Horizontal heat flows and cloud cover on Earth
- Ocean thermohaline circulation
- Mantle convection
- Evolutionary optimisation of ATP synthase

Summary

- Maximum entropy: A method of inferring distribution of characteristics in a complex system at equilbrium. Only knowledge needed is those system constraints required to obtain reproducible results.
- Maximum entropy production: An analogous (though more controversial) method for complex systems out of equilbrium (though still in a steady state)