ISC 5228
Markov Chain Monte Carlo
In-class Assignment

Boltzmann Distribution

In statistical physics, the Boltzmann distribution gives the probability that a system will be in a certain state ($\mathbf{s}$) in terms of the energy $E(\mathbf{s})$ and absolute temperature T as,[1]

$$\pi(\mathbf{s}) \propto e^{-E(\mathbf{s})/T} \tag{1}$$

Consider a simple harmonic oscillator.

$$E(s) = \frac{1}{2}s^2 \tag{2}$$

This may be a crude model for a diatomic molecule like hydrogen (say).

1. For $T = 1$, sketch the Boltzmann probability distribution corresponding to eqn (2).
2. Overlay, $\pi(s)$ corresponding to $T = 1/2$ and $T = 2$ on the sketch above.
3. Extrapolate these observations and speculate about the shape of $\pi(s)$ for $T = 0$ and $T \to \infty$.
4. **Hastings ratio**: Consider two states s_1 and s_2. What is the ratio of the probabilities, $\pi(s_2)/\pi(s_1)$.
5. Now, let us go back to the general case eqn (1). Consider two states $\mathbf{s}_1$ and $\mathbf{s}_2$ with corresponding energies E_1 and E_2. Show that the ratio of the probabilities

$$\frac{\pi(\mathbf{s}_2)}{\pi(\mathbf{s}_1)} = e^{-\Delta E/T} \tag{3}$$

where $\Delta E = E_2 - E_1$.

[1]It can be derived by maximizing entropy under the constaint of a mean energy value. In eqn (1), I assume that the Boltzman constant $k_B = 1$.