

Maximizing the Entropy predicts flat distributions when there are no constraints (beyond normalized probability distributions).

We want to maximize $S(p_1, p_2, \dots, p_t) = -k \sum_{i=1}^t p_i \ln p_i$

But we have a normalization

Constraint: $g(p_1, p_2, \dots, p_t) = \left(\sum_{i=1}^t p_i \right) - 1 = 0$

We create a new objective function:

$$F = S - \alpha g \quad \leftarrow \text{Lagrange Multiplier}$$

And minimize F :

$$\frac{\partial F}{\partial p_i} = \frac{\partial S}{\partial p_i} - \alpha \frac{\partial g}{\partial p_i} = 0 \quad \leftarrow \text{minimizes } F$$

Let's figure out these partials:

$$\frac{\partial g}{\partial p_i} = \frac{\partial}{\partial p_i} \left(\sum_{i=1}^t p_i - 1 \right)$$

$$= \frac{\partial}{\partial p_i} (p_1 + p_2 + p_3 + \dots + p_t - 1)$$

$$= 1 \quad \leftarrow \text{no matter which } p_i$$

$$\frac{\partial S}{\partial p_i} = \frac{\partial}{\partial p_i} \left(-k \sum_{i=1}^t p_i \ln p_i \right)$$

$$= -k \left(p_i \frac{\partial}{\partial p_i} (\ln p_i) + \frac{\partial p_i}{\partial p_i} \ln p_i \right)$$

$$= -k \left(\frac{p_i}{p_i} + \ln p_i \right)$$

$$= -k (1 + \ln p_i)$$

(3-2)

Now, we can put them together

$$\frac{\partial F}{\partial p_i} = -k - k \ln p_i - \alpha = 0$$

$$\ln p_i = \frac{-\alpha - k}{k} = -\frac{\alpha}{k} - 1$$

$$p_i = e^{-(\alpha/k + 1)}$$

What does this mean for the relative probabilities?

$$\frac{p_i}{\sum_{i=1}^t p_i} = \frac{e^{-(\alpha/k + 1)}}{\sum_{i=1}^t \underbrace{(e^{-(\alpha/k + 1)})}_{\text{all of these are the same!}}} = \frac{e^{-(\alpha/k + 1)}}{t (e^{-(\alpha/k + 1)})} = \frac{1}{t}$$

All of the p_i are the same $\rightarrow$ flat distribution

Maximizing the entropy predicts exponential distributions when there are constraints.

Suppose we roll a t -sided die N times

$$p_i = \frac{n_i}{N}$$

Now, let's assign a "score" to each side, ε_i

Total score:

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

Average score / roll:

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

What is the distribution that maximizes the entropy and is consistent with an observed average score?

Now we have two constraints:

$$g(p_1, p_2, \dots, p_t) = \sum_{i=1}^t p_i - 1 = 0$$

$$h(p_1, p_2, \dots, p_t) = \sum_{i=1}^t p_i \epsilon_i - \langle E \rangle = 0$$

So our new objective function has 2 undetermined multipliers:

$$F = S - \alpha g - k \beta h$$

this k is just here for convenience

Like before, we have

$$\frac{\partial g}{\partial p_i} = 1$$

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

$$\frac{\partial h}{\partial p_i} = \epsilon_i$$

So:

$$\frac{\partial F}{\partial p_i} = -k - k \ln p_i - \alpha - k \beta \epsilon_i = 0$$

$$-k \ln p_i = \cancel{4/4} k + \alpha + k \beta \epsilon_i$$

$$\ln p_i = -1 - \frac{\alpha}{k} - \beta \epsilon_i$$

$$p_i = e^{-1 - \frac{\alpha}{k} - \beta \epsilon_i} = e^{-(1 + \frac{\alpha}{k})} e^{-\beta \epsilon_i}$$

The relative probabilities

$$\frac{p_i}{\sum_i p_i} = \frac{e^{-(1 + \frac{\alpha}{k})} e^{-\beta \epsilon_i}}{\sum_i e^{-(1 + \frac{\alpha}{k})} e^{-\beta \epsilon_i}} = \frac{e^{-\beta \epsilon_i}}{\sum_{i=1}^t e^{-\beta \epsilon_i}}$$

(3-4)

This is the Boltzmann distribution law:

$$p_i = \frac{e^{-\beta \epsilon_i}}{\sum_{i=1}^t e^{-\beta \epsilon_i}}$$

← the "score" ϵ_i is just the energy associated with a state

The denominator is so important, we call it the partition function:

$$q = \sum_{i=1}^t e^{-\beta \epsilon_i}$$

$$\langle E \rangle = \sum_{i=1}^t \epsilon_i p_i = \frac{1}{q} \sum_{i=1}^t \epsilon_i e^{-\beta \epsilon_i}$$

Let's do an example with a biased coin:

$$t=2$$

$$\epsilon_H = 2$$

$$\epsilon_T = 1$$

← heads are more valuable

(For an unbiased coin, $P_H = P_T = \frac{1}{2}$ and $\langle E \rangle = \frac{3}{2}$)

Using the Boltzmann distribution, however:

$$P_T = \frac{e^{-\beta(1)}}{e^{-\beta(1)} + e^{-\beta(2)}} = \frac{x}{x + x^2} \quad \text{where } x = e^{-\beta}$$

$$P_H = \frac{e^{-\beta(2)}}{e^{-\beta(1)} + e^{-\beta(2)}} = \frac{x^2}{x + x^2}$$

$$\langle E \rangle = (1)P_T + (2)P_H = \frac{x + 2x^2}{x + x^2} = \frac{1 + 2x}{1 + x}$$

(3-5)

Solving for x gives:

$$x = \frac{\langle E \rangle - 1}{2 - \langle E \rangle}$$

If you observe that $\langle E \rangle = \frac{3}{2}$, then $x = 1$
and $P_H = P_T = \frac{1}{2}$ as expected (unbiased).

If instead, you observe $\langle E \rangle = 1.2$, then $x = \frac{1}{4}$
and $P_H = \frac{1}{5}$ with $P_T = \frac{4}{5}$ (biased).