

Exercise 1. Rényi entropies

One Schur-concave function you are already familiar with is the Shannon entropy. The Shannon entropy can be generalized to the Rényi entropies, defined for a vector of probabilities p :

$$S_\alpha(p) := -\frac{1}{\alpha-1} \log \sum_{i=1}^m p_i^\alpha \quad (\alpha \in \mathbb{R}^+ \setminus \{0, 1\}),$$

with a few special cases corresponding to $\alpha \in \{0, 1, \infty\}$:

$$\begin{aligned} S_0(p) &:= \log \text{rank } p && (\text{max entropy}), \\ S_1(p) &:= -\sum_{i=1}^m p_i \log p_i && (\text{Shannon entropy}), \\ S_\infty(p) &:= -\log \max_i p_i && (\text{min entropy}). \end{aligned}$$

Show that:

(a) The definitions of three special cases are consistent with the general formula:

$$\begin{aligned} \lim_{\alpha \rightarrow 0} S_\alpha &= S_0, \\ \lim_{\alpha \rightarrow 1} S_\alpha &= S_1, \\ \lim_{\alpha \rightarrow \infty} S_\alpha &= S_\infty. \end{aligned}$$

Solution The max entropy:

$$\lim_{\alpha \rightarrow 0} S_\alpha = -\lim_{\alpha \rightarrow 0} \frac{1}{\alpha-1} \log \sum_{i=1}^m p_i^\alpha = \log \sum_{i=1, p_i \neq 0}^m 1 = \log \text{rank } p.$$

The Shannon entropy (here we use the L'Hôpital's rule for calculating limits $\lim_{\alpha \rightarrow 1} \frac{f(\alpha)}{g(\alpha)} = \lim_{\alpha \rightarrow 1} \frac{f'(\alpha)}{g'(\alpha)}$ for $\lim_{\alpha \rightarrow 1} f(\alpha) = \lim_{\alpha \rightarrow 1} g(\alpha) = 0$):

$$\lim_{\alpha \rightarrow 1} S_\alpha = -\lim_{\alpha \rightarrow 1} \frac{1}{\alpha-1} \log \sum_{i=1}^m p_i^\alpha = -\lim_{\alpha \rightarrow 1} \log \sum_{i=1}^m p_i^\alpha \log p_i = -\sum_{i=1}^m p_i \log p_i.$$

The min entropy (wlog suppose that $\max_i p_i = p_1$):

$$\lim_{\alpha \rightarrow \infty} S_\alpha = -\lim_{\alpha \rightarrow \infty} \frac{1}{\alpha-1} \log \sum_{i=1}^m p_i^\alpha = -\lim_{\alpha \rightarrow \infty} \frac{1}{\alpha-1} \left(\alpha \log p_1 + \log \left(1 + \frac{p_2^\alpha}{p_1^\alpha} \right) \right) = -\log p_1 = -\log \max_i p_i.$$

(b) All Rényi entropies are Schur-concave.

Solution We just check the Schur-Ostrowski criterion:

$$(p_i - p_j)(-p_i^{\alpha-1} + p_j^{\alpha-1}) \leq 0.$$

(c) All Rényi entropies have values between 0 (for a pure distribution) and $\log m$ (for a maximally mixed distribution), where m is the size of the system.

Solution S_α is non-increasing in α for any given probability vector p , which can be shown by differentiation: an easy way to see why is to observe that $\frac{dS_\alpha}{d\alpha}$ is proportional to relative entropy, which is always positive. Hence,

$$0 \leq S_\infty \leq S_\alpha \leq S_0 \leq \log m.$$

Now let us define the relative Rényi entropies as

$$S_\alpha(p||q) := \frac{\text{sgn}(\alpha)}{\alpha - 1} \log \sum_{i=1}^m p_i^\alpha q_i^{1-\alpha} \quad (\alpha \in \mathbb{R} \setminus \{1\}),$$

where we set $0^0 := 0$, and $\text{sgn}(\alpha) = \begin{cases} +1 & \text{if } \alpha \in [0, +\infty] \\ -1 & \text{if } \alpha \in [-\infty, 0). \end{cases}$

(d) Show that $\lim_{\alpha \rightarrow 1} S_\alpha(p||q) = S(p||q)$, where $S(p||q)$ is the usual conditional entropy, $S(p||q) = -\sum_{i=1}^m p_i \log \frac{p_i}{q_i}$.

Solution Here, the proof goes similar to what we did for Shannon entropy in part (a).

Exercise 2. Thermal operations with restrictions

One of the important quantities at macroscopic scale is (Helmholz) free energy:

$$F(\rho) = E(\rho) - TS(\rho).$$

At constant ambient temperature T and constant volume, transitions between two states are possible if and only if the difference between the free energies of the initial and the final states is negative. This free-energy difference also tells us how much work we can extract, or need to invest, during a thermodynamic state transition.

At the microscopic scale, however, the possibility of state transitions is not determined by free energy alone, but by an infinite family of free-energy-like quantities. These known results rely crucially on the assumption that the thermal machine is not only exactly preserved in every cycle but also kept uncorrelated from the quantum systems on which it acts:

$$\rho_A \otimes \sigma_M \mapsto \rho'_A \otimes \sigma_M$$

We assume that the machine can strictly only perform the following operations: energy-preserving unitaries; accessing thermal states from the bath; and ignoring heat bath degrees of freedom by tracing over them (thermal operations). If we assume for the moment that there is no work reservoir W , and demand that these operations preserve the local state of the machine M and also its independence from A , then they describe transitions $\rho_A \rightarrow \rho'_A$. It has been shown [1] that a thermal transformation can achieve this transition (up to an arbitrarily small error on A) if and only if all α -free energies decrease in the process:

$$\Delta F_\alpha = F_\alpha(\rho'_A) - F_\alpha(\rho_A) \leq 0 \text{ for all } \alpha \geq 0. \quad (1)$$

Here $F_\alpha(\rho_A) = k_B T S_\alpha(\rho_A || \gamma_A) - k_B T \log Z_A$, with Z_A the partition function of A , T the background temperature, k_B Boltzmann's constant, and S_α the Rényi divergence of order α (see previous exercise). For $\alpha \in \{-\infty, 0, 1, \infty\}$, we use the definitions

$$S_0(p||q) = \lim_{\alpha \searrow 0} S_\alpha(p||q) = -\log \sum_{i:p_i \neq 0} q_i, \quad S_1(p||q) \equiv S(p||q),$$

$$S_\infty(p||q) = \lim_{\alpha \rightarrow \infty} S_\alpha(p||q) = \log \max_i \frac{p_i}{q_i}, \quad S_{-\infty}(p||q) = \lim_{\alpha \rightarrow -\infty} S_\alpha(p||q) = S_\infty(q||p).$$

(a) For $\alpha = 1$, show that the free energy reduces to the Helmholtz free energy $F_1 = F$.

Here, we look at general transformations of the form:

$$\rho_A \otimes \sigma_M \mapsto \sigma_{AM}, \text{ with } \text{tr}_M(\sigma_{MA}) = \rho'_A \text{ and } \text{tr}_A(\sigma_{MA}) = \sigma_M.$$

To see that the α -free energies impose severe constraints on the workings of a thermal machine, let us look at a simple example.

(b) Suppose that a thermal machine is supposed to heat up a system A from its thermal state γ_A to infinite temperature (a fully mixed state). Suppose that A is a qubit with energies 0 and E_A , its initial temperature is such that $\beta E_A = \log 2$. The associated work cost will be delivered by an additional work bit W with energy gap $\Delta > 0$. It starts in its excited state $|e\rangle$ and will end up in its ground state $|g\rangle$. The machine implements the transition

$$\gamma_A \otimes |e\rangle\langle e|_W \mapsto \rho'_A \otimes |g\rangle\langle g|_W$$

with a work cost Δ that is as small as possible. As before, this is achieved by a catalytic thermal operation of the form

$$\gamma_A \otimes \sigma_M \otimes |e\rangle\langle e|_W \mapsto \rho'_A \otimes \sigma_M \otimes |g\rangle\langle g|_W$$

Calculate the α -energy difference for $\alpha \rightarrow \infty$. For which work bit gaps Δ is this difference ≤ 0 for all α ? Compare this case to the usual free energy difference ($\alpha = 1$).

Solution The initial thermal state is $\gamma_A = \begin{pmatrix} 2/3 & 0 \\ 0 & 1/3 \end{pmatrix}$. The desired target state is $\rho'_A = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$. The α -free energy difference between initial and final state of AW turns out to be

$$\frac{\Delta F_\alpha}{k_B T} = \frac{\log(2^{1-\alpha} + 1) - \alpha \log 2 + (\alpha - 1) \log 3}{\alpha - 1} - \frac{\Delta}{k_B T}$$

which is increasing in α . Thus, this is ≤ 0 for all α if and only if $\Delta F_\infty \leq 0$, which becomes

$$\Delta \geq k_B T \log(3/2) \approx .4 k_B T.$$

This is the ultimate limit for a transition to be successfully implementable. On the other hand, the standard free energy difference is $\Delta F/(k_B T) = \log 3 - 3/2 \log 2 - \Delta/(k_B T)$, and for this to be ≤ 0 we must have

$$\Delta \geq k_B T (\log 3 - 3/2 \log 2) \approx .06 k_B T.$$

Thus, textbook thermodynamic reasoning would suggest that $.06 k_B T$ of energy should be sufficient for the state transition; however, our analysis has shown that the machine needs to spend considerably more work, namely $.4 k_B T$. As explained above, one reason for this is that we are dealing with the case of a *single* system only. The standard thermodynamic equations apply to large numbers of (independent, or weakly correlated) identical systems and their averages.

One reason for the discrepancy is that we are dealing with the case of a single system only. Intuitively, by acting collectively on a large number of particles, a machine can achieve more than if it had to act on each particle separately.

We thus have two independent motivations to allow correlations between M and AW : the difficulty to avoid correlations on interaction, and the desire to achieve higher efficiency. We will now show that the latter goal can indeed be achieved by allowing correlations to build up, even if the catalyst M is as small as a single qubit.

Let us now enforce thermal transitions of the form

$$\gamma_A \otimes \sigma_M \otimes |e\rangle\langle e|_W \longrightarrow \rho'_{AM} \otimes |g\rangle\langle g|_W,$$

- (c) Suppose that M has a trivial Hamiltonian, $H_M = 0$, and two basis states $|0\rangle$ and $|1\rangle$ (both of energy zero). Denote ground and excited state of A by $|g_A\rangle$ and $|e_A\rangle$. Consider a correlated state of A and M

$$\begin{aligned} \rho'_{AM} &:= \frac{1}{10}|g_A0\rangle\langle g_A0| + \frac{4}{10}|g_A1\rangle\langle g_A1| \\ &\quad + \frac{2}{10}|e_A0\rangle\langle e_A0| + \frac{3}{10}|e_A1\rangle\langle e_A1|. \end{aligned}$$

What are the reduced states of A (ρ'_A) and M (σ_M)?

Solution By computing the partial trace, we find that ρ'_A is indeed the infinite-temperature state, and

$$\rho'_M = \frac{3}{10}|0\rangle\langle 0| + \frac{7}{10}|1\rangle\langle 1| =: \sigma_M$$

which will also be our local qubit catalyst state σ_M .

- (d) Now enforce the thermal transition of a form

$$\gamma_A \otimes \sigma_M \otimes |e\rangle\langle e|_W \longrightarrow \rho'_{AM} \otimes |g\rangle\langle g|_W.$$

How much work do we need to spend on this process? Compare with the value given by assuming a catalytic transition.

Hint: Use Lorenz curves. You can take advantage of Matlab or Mathematica, too.

Solution Our goal is to determine under what conditions the transition

$$\gamma_A \otimes \sigma_M \otimes |e\rangle\langle e|_W \longrightarrow \rho'_{AM} \otimes |g\rangle\langle g|_W \tag{S.1}$$

can be accomplished by a thermal operation, without additional catalyst. Labelling (and sorting) the eigenvectors of AMB by

$$|g_A0g\rangle, |g_A0e\rangle, |g_A1g\rangle, |g_A1e\rangle, |e_A0g\rangle, |e_A0e\rangle, |e_A1g\rangle, |e_A1e\rangle,$$

the state on the left-hand side corresponds to the probability distribution

$$p_{AMW} = \left(0, \frac{1}{5}, 0, \frac{7}{15}, 0, \frac{1}{10}, 0, \frac{7}{30}\right),$$

and the state on the right-hand side to

$$q_{AMW} = \left(\frac{1}{10}, 0, \frac{2}{5}, 0, \frac{1}{5}, 0, \frac{3}{10}, 0\right).$$

The sorted energy eigenvalues are

$$(E_1, \dots, E_8) = (0, \Delta, 0, \Delta, E_A, E_A + \Delta, E_A, E_A + \Delta),$$

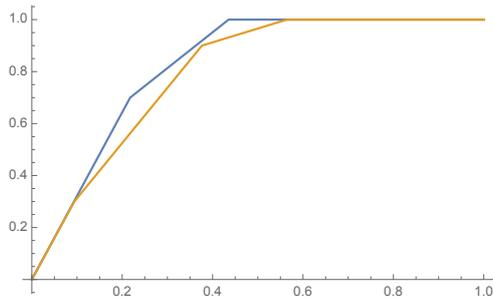


Figure 1: The thermal Lorenz curves signify the possibility of state transition by a thermal operation [2].

where $E_A = k_B T \log 2$. We use the thermomajorization criterion: there exists a thermal operation mapping p to q if and only if the thermal Lorenz curve of p is everywhere on or above the thermal Lorenz curve of q . Using Mathematica, we have generated the plots in Figure 1 for $\Delta = .26k_B T$, which shows that p 's curve (in blue) is indeed nowhere below q 's curve (in orange); the same must then be true for larger values of Δ (and we have numerically verified this). We have also used Mathematica to verify directly the necessary inequalities for all “elbow points” of the curves.

That is, the single qubit catalyst allows us to save about 1/3 of the total work cost as compared to previous result.

It can be shown that only the standard Helmholtz free energy condition $\Delta F_1 \equiv \Delta F \leq 0$ survives as a relevant necessary condition for a correlating state transition. For details, please consult [2].

References

- [1] F. Brandão, M. Horodecki, N. Ng, J. Oppenheim, and S. Wehner, *The Second Laws of Quantum Thermodynamics*. **Proc. Natl. Acad. Sci. U.S.A.** **112**, 3275 (2015).
- [2] Markus P. Müller, *Correlating Thermal Machines and the Second Law at the Nanoscale*. **Physical Review X**, **8**(4) (2018).