Systematically understanding the power of small catalysts Student: Chong Bi Qi Supervisor: Assoc Prof Nelly Ng Huei Ying



Division of School of Physical and Mathematical Sciences

Abstract

Many stochastic processes in thermodynamics and information processing can be studied in the language of state transitions, in particular using majorization conditions. Interestingly, catalysts can also be used to facilitate state transition, enabling extra processes that were otherwise not possible. However, most studies are concerned about high dimension catalysts, and little is understood about the construction of simple catalys states. This project aims to explore the power of small catalysts and find a way to construct simple catalysts.

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Majorization

Majorization is used to determine if the transition between two states is possible[1]. Let $x = (x_1, \ldots, x_d)$ and $y = (y_1, \ldots, y_d) \in \mathbb{R}^d$ be ddimensional probability vectors with their components arranged in nonincreasing order. In other words, $x_1 \ge x_2 \ge \ldots \ge x_d$ and $y_1 \ge y_2 \ge \ldots \ge x_d$

The approach

Given $x_1, x_2, y \in \mathbb{R}^4, z_1, z_2 \in \mathbb{R}^2$ such that $x_i \not\prec y$ but $x_i \otimes z_i \prec y \otimes z_i$ (i = 1)or 2), x_{λ}, z_{λ} follow the previous notation. Note that $\vec{\varepsilon_i}$ and $\vec{\varepsilon_2}$ is the vector that determines x_1, x_2 repectively. Let $\vec{\varepsilon_{\lambda}} = \Gamma_{\lambda}(\vec{\varepsilon_1}, \vec{\varepsilon_2})$, hence M'_{λ} and m'_{λ} depend on $\vec{\varepsilon}_{\lambda}$. Then, the graphs of p agaisst λ can be plotted as below.

 y_d . x is said to be majorized by y, written $x \prec y$, if:

$$\sum_{i=1}^{l} x_i \le \sum_{i=1}^{l} y_i \qquad (1 \le l < d)$$

Since both x and y are probability vectors, $\sum_{i=1}^{d} x_i = \sum_{i=1}^{d} y_i = 1$. If x is not majorized by y, it is written as $x \not\prec y$. A catalyst, z, is a state that allow y to majorize x if it is added into the system. Namely: $x \not\prec y$ but $x \otimes z \prec y \otimes z$. If there exist such a z, x is said to be trumped by y, written $x \prec_T y$.

Study shows that $x \prec y$ if $x \prec_T y$ for all states smaller than 4 dimensions [1]. Since x is already majorized by y, there is no need for catalyst. Therefore, the project focuses on studying 4 dimension states with 2 dimension catalysts, which is the smallest dimension where a catalyst starts to be useful.

Convexity and simple catalyst

Let $T_2(y)$ denote the set of vectors x such that $x \otimes z \prec y \otimes z$ is possible for some z = (p, 1 - p). Next, we introduce the mixing operation, which indicate the linear interpolation between two variables.



Figure 2: M' not convex Figure 1: M' and m' convex The red vertical line represent the set of z that can catalyze the respective x and y pairs. m'_{λ} and M'_{λ} shows the lower and upper boundary of the catalyst when x_{λ} varies across 0 to 1. $p_{mc} := \Gamma_{\lambda}(m'_1, m'_2)$ and $p_{Mc} := \Gamma_{\lambda}(M'_1, M'_2)$ is the linear interpolation of m'_1, m'_2 and M'_1, M'_2 . A catalyst z_{λ} is said to be convex if the linear interpolation of z_1, z_2 can catalyse x_{λ} and y. In other words, if z_{λ} is within the bound of m'_{λ} and M'_{λ} , then it is convex. Thus, we define the following:

1. the upper bound of the catalyst is convex if $m'_{\lambda} \geq p_{mc}$.

2. the lower bound of the catalyst is convex if $M'_{\lambda} \leq p_{Mc}$.

for all $\lambda \in [0,1]$. Numerical result shows that covexity over m' and M' is independent. Therefore we can analysize them separately. For M', $\mu_b \leq p_{mc}$, and μ_a is always the cause if M_{λ} is not convex. We then derive the following:

 $\Gamma_{\lambda}(a,b) := (1-\lambda)a + \lambda b, \quad \text{for all } \lambda \in [0,1].$ (2)

Given two vectors $x_1, x_2 \in T_2(y)$, we define the mixture of x_1, x_2 and z_1, z_2 as $x_{\lambda} := \Gamma_{\lambda}(x_1, x_2)$ and $z_{\lambda} := \Gamma_{\lambda}(z_1, z_2)$. It is known that $T_2(y)$ is convex[1], therefore $x_{\lambda} \in T_2(y)$. However, the convexity of cataysts is unkown. In other words, even though it is known that x_{λ} can be majorized by y with some 2D catalyst, it is unsure if $x_{\lambda} \otimes z_{\lambda} \prec \text{or} \not\prec y \otimes z_{\lambda}$. It is only known that $x_{\lambda} \otimes z_1 \otimes z_2 \prec y \otimes z_1 \otimes z_2$, but this could greatly increase the dimension and complexity of the system. This project review the convexity of the set of catalyst that catalysize x_{λ} , and outlined the condition when a simple mixing on the catalyst is sufficient for $x_{\lambda} \otimes z_{\lambda} \prec y \otimes z_{\lambda}$.

Anspach condition

Let $y = (y_1, y_2, y_3, y_4), x = (x_1, x_2, x_3, x_4), z = (p, 1 - p)$ (p > 0.5). Anspach shows that for $x \not\prec y$ but $x \otimes z \prec y \otimes z$, there should be a vector $\vec{\varepsilon} = (\varepsilon_1, \varepsilon_2, \varepsilon_3)$ such that:

Theorem 1 (Anspach)

(3) $y_1 = x_1 + \varepsilon_1$ (4) $y_2 = x_2 - \varepsilon_2 - \varepsilon_3$

1.
$$\gamma(\lambda) := \mu_a + \lambda(M'_1 - M'_2)$$

2. if $\gamma(\lambda) \leq M'_1$ for all $\lambda \in [0,1]$, then the lower boundary of catalyst is convex.

Conclusion

Using the analysis above, we develop an algorithm that examine the convexity of the catalyst over the lower boundary of p (or M').



$$y_{3} = x_{3} + \varepsilon_{2} + \varepsilon_{3}$$

$$y_{4} = x_{4} - \varepsilon_{3}$$

$$\varepsilon_{1}, \varepsilon_{2} > 0, \quad \varepsilon_{3} \ge 0$$

and $M' \leq p \leq m'$

$$m' = \min(\frac{\varepsilon_1}{\varepsilon_1 + \varepsilon_2}, 1 - \frac{y_4}{y_3 + y_4 - \varepsilon_2}, \frac{y_1}{y_1 + y_2 + \varepsilon_2})$$
(8)

$$M' = \max(\mu_a, \mu_b)$$
(9)
where $\mu_a = \frac{\varepsilon_2}{\varepsilon_2 + \varepsilon_3}, \quad \mu_b = \frac{y_2 + \varepsilon_2}{y_2 + y_3}$ (10)

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Figure 3: LC indicate the catalyst is linearly convex over M'.

In short, the convexity of catalyst is achievable under a series of conditions, and the specific algorithm for M' to be convex is provided.

References

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