Article

Entropic Distance for Nonlinear Master Equation

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Abstract: More and more works deal with statistical systems far from equilibrium, dominated by unidirectional stochastic processes augmented by rare resets. We analyze the construction of the entropic distance measure appropriate for such a dynamics. We demonstrate that a power-like nonlinearity in the state probability in the master equation naturally leads to the Tsallis (Havrda–Charvát, Aczél–Daróczy) q-entropy formula in the context of seeking for the maximal entropy state at stationarity. A few possible applications of a certain simple and linear master equation to phenomena studied in statistical physics are listed at the end.

Keywords: q-entropy; entropic distance; Matthew principle

1. Definition and Properties of Entropic Distance

Entropic distance, more properly called "entropic divergence", is traditionally interpreted as a relative entropy, as a difference between entropies with a prior condition and without [1]. It is also the Boltzmann–Shannon entropy of a distribution relative to another [2]. Looking at this construction, however, from the viewpoint of a generalized entropy [3], the simple difference or logarithm of a ratio cannot be hold as a definition any more.

Instead, in this paper, we explore a reverse engineering concept: seeking for an entropic divergence formula at the first place, which is subject to some wanted properties, we consider entropy as a derived quantity. More precisely we seek for entropic divergence formulas appropriate to a given stochastic dynamics, shrinking during the approach to a stationary distribution, whenever it exists, and establish the entropy formula from this distance to the uniform distribution. By doing so we serve two goals: i) having constructed a non-negative entropic distance we derive an entropy formula which is maximal for the uniform distribution, and ii) we come as near as possible to the classical difference formula for the relative entropy.

We start our discussion by contrasting the definition of the metric distance, knwon from geometry, to the basic properities of an entropic distance. The metric distance posesses the following properties:

1. $\rho(P,Q) \geq 0$ for a pair of points P and Q,
2. $\rho(P,Q) = 0$ only for $P = Q$,
3. $\rho(P,Q) = \rho(Q,P)$ symmetric measure,
4. $\rho(P,Q) \leq \rho(P,R) + \rho(R,Q)$, the triangle inequality in elliptic spaces.

The entropic divergence on the other hand is neither necessarily symmetric, nor can satisfy a triangle inequality. On the other hand it is subject to the second law of thermodynamics, distingusihing the time arrow from the past to the future. We require for a real functional, $\rho[P,Q]$, depending on the distributions P_n and Q_n, the followings to hold:

1. $\rho[P,Q] \geq 0$ for a pair of distributions P_n and Q_n,
2. $\rho[P,Q] = 0$ only if the distributions coincide $P_n = Q_n$,
3. $\frac{\mathrm{d}}{\mathrm{d}t}\rho[P,Q] \leq 0$ if Q_n is the stationary distribution,
4. $\frac{\mathrm{d}}{\mathrm{d}t}\rho[Q,Q] = 0$ only for $P_n = Q_n$, i.e. the stationary distribution is unique.

Although this definition is not symmetric in the handling of the normalized distributions P_n and Q_n, it is an easy task to consider the symmetrized version, $s[P,Q] \equiv \rho[P,Q] + \rho[Q,P]$. This symmetrized entropic divergence inherits some properties from the fiducial construction. Considering a scaling trace form entropic divergence, $\rho[P,Q] = \sum\limits_n \sigma(\xi_n)\, Q_n$ with $\xi_n = P_n/Q_n$, to begin with, we identify the following symmetrized kernel function:

$$\mathfrak{s}(\xi) := \sigma(\xi) + \xi\, \sigma(1/\xi). \tag{1}$$

The only constraint is to start with a core function, $\sigma(\xi)$ with a definite concavity. Jensen inequality tells for $\sigma'' > 0$ that

$$\sum_n \sigma(\xi_n)\, Q_n \geq \sigma\left(\sum_n \xi_n Q_n\right) = \sigma\left(\sum_n P_n\right) = \sigma(1). \tag{2}$$

For satisfying property 1 and 2 one simply sets $\sigma(1) = 0$. Interesting enough, but this setting suffices also for the satsifaction of the second law of thermodynamics, formulated above as further constraints 3 and 4. As a consequence of the symmetrization it also follows that $\mathfrak{s}(1) = 0$ and $\mathfrak{s}'' > 0$.

The symmetrized entropic divergence shows some new, emergent properties. We list its derivatives as follows:

$$\begin{aligned}
\mathfrak{s}(\xi) &= \sigma(\xi) + \xi\, \sigma(1/\xi) \\
\mathfrak{s}'(\xi) &= \sigma'(\xi) + \sigma(1/\xi) - \frac{1}{\xi}\sigma'(1/\xi) \\
\mathfrak{s}''(\xi) &= \sigma''(\xi) - \cancel{\frac{1}{\xi^2}\sigma'(1/\xi)} + \cancel{\frac{1}{\xi^2}\sigma'(1/\xi)} + \frac{1}{\xi^3}\sigma''(1/\xi).
\end{aligned} \tag{3}$$

The consequences, listed below, can be derived from these general relations:

1. $\mathfrak{s}(1) = 2\,\sigma(1) = 0,$
2. $\mathfrak{s}'(1) = \sigma(1) = 0,$
3. $\mathfrak{s}'' > 0 \quad \Rightarrow \quad \xi_m = 1$ is a minimum,
4. $\mathfrak{s}(\xi) \geq 0.$

In this way the kernel function and hence each summand in the symmetrized entropic divergence formula is non-negative, not only the total sum.

2. Entropic distance evolution due to linear stochastic dynamics

Now we study properties 3 and 4, by evaluating the rate of change of the entropic divergence in time. This change is based on the dynamics (time evolution) of the evolving distribution, $P_n(t)$, while the targeted stationary distribution, Q_n is by definition time independent. First we consider a class of stochastic evolutions governed by differential equations for $\dot{P}_n(t) \equiv \frac{\mathrm{d}P_n}{\mathrm{d}t}$, linear in the distribution, $P_n(t)$ [4]. We consider the trace form $\rho[P,Q] = \sum\limits_n Q_n\, \sigma\left(\frac{P_n}{Q_n}\right)$ and the background master equation

$$\dot{P}_n = \sum_m \left(w_{nm} P_m - w_{mn} P_n\right). \tag{4}$$

The antisymmetrized sum in the above equation is merely to ensure the conservation of the norm, $\sum\limits_n P_n = 1$, during the time evolution. Using again the notation $\xi_n = P_n/Q_n$ we obtain

$$\dot{\rho} \;=\; \sum_n \sigma'(\xi_n)\,\dot{P}_n \;=\; \sum_{n,m} \sigma'(\xi_n)\;(w_{nm}\,\xi_m Q_m - w_{mn}\,\xi_n Q_n)\,. \tag{5}$$

The basic trick is to apply the splitting $\xi_m = \xi_n + (\xi_m - \xi_n)$ to get

$$\dot{\rho} \;=\; \sum_n \sigma'(\xi_n)\,\xi_n \cancel{\sum_m (w_{nm}\,Q_m - w_{mn}\,Q_n)} + \sum_{n,m} \sigma'(\xi_n)(\xi_m - \xi_n) w_{nm}\,Q_m. \tag{6}$$

Here the sum in the first term vanishes due to the very definition of the stationary distribution, Q_n. For estimating the remaining term we utilize the Taylor series remainder theorem in the Lagrange form. We recall the Taylor expansion of the kernel function $\sigma(\xi)$,

$$\sigma(\xi_m) \;=\; \sigma(\xi_n) + \sigma'(\xi_n)(\xi_m - \xi_n) + \frac{1}{2}\sigma''(c_{mn})(\xi_n - \xi_m)^2, \tag{7}$$

with $c_{mn} \in [\xi_m, \xi_n]$. Here the first derivative term has occured in eq.(6). This construction delivers

$$\dot{\rho} \;=\; \cancel{\sum_{n,m} [\sigma(\xi_m) - \sigma(\xi_n)]\, w_{nm} Q_m} - \frac{1}{2}\sum_{n,m} \sigma''(c_{mn})\,(\xi_m - \xi_n)^2\, w_{nm} Q_m. \tag{8}$$

Here the first sum vanishes again: after exchanging the indices m and n in the first summand, the result is proportional to the total balance expression, which is zero for the stationary distribution. With positive transition rates, $w_{nm} > 0$ the approach to stationary distribution, $\dot{\rho} \le 0$ is hence proven for all $\sigma'' > 0$. We note that we never used the detailed balance condition for the transition rates, only the vanishing of the total balance, which defines the stationary distribution.

This proof, without recalling the detailed balance condition as Boltzmann's famous H-theorem did, is quite general. Any core function with positive second derivative and the scaling trace form co-act to ensure the correct change in time. By using the traditional choice, $\sigma(\xi) = -\ln \xi$, we have $\sigma' = -1/\xi$ and $\sigma''(\xi) = 1/\xi^2 > 0$, satisfying indeed all requirements. The integrated entropic divergence formula (no symmetrization) in this case is given as the Kullback–Leibler divergence :

$$\rho[P,Q] \;=\; \sum_n Q_n \,\ln \frac{Q_n}{P_n}. \tag{9}$$

There is a rationale behind using the logarithm function. It is the only one being additive for the product form of its argument, mapping factorizing and hence statistically independent distributions to an additive entropic divergence kernel: For $P_n^{(12)} = P_n^{(1)} P_n^{(2)}$ also $Q_n^{(12)} = Q_n^{(1)} Q_n^{(2)}$ therefore we have $\xi_n^{(12)} = \xi_n^{(1)} \xi_n^{(2)}$. Aiming at $\sigma(\xi^{(12)}) = \sigma(\xi^{(1)}) + \sigma(\xi^{(2)})$, the solution is $\sigma(\xi) = \alpha \ln \xi$. For $\sigma'' > 0$ it must be $\alpha < 0$, so without restricting generality one chooses $\alpha = -1$.

Finally we would like to treat this entropic divergence as an entropy difference. This is achieved when comparing the stationary distribution to the uniform distribution, $U_n = 1/W, n = 1, 2, \ldots W$. Using the above Kullback–Leibler divergence formula one easily derives

$$\rho[U,Q] \;=\; \sum_{n=1}^{W} Q_n \ln(W Q_n) \;=\; \ln W + \sum_n Q_n \ln Q_n \;=\; S_{BG}[U] - S_{BG}[Q] \tag{10}$$

with

$$S_{BG}[Q] \;=\; -\sum_n Q_n \,\ln Q_n, \tag{11}$$

being the Boltzmann–Gibbs–Planck–Shannon entropy formula. From the Jensen inequality it follows $\rho(U,Q) \ge 0$, so $S_{BG}[U] \ge S_{BG}[Q]$.

62 **3. Entropic divergence evolution for nonlinear master equations**

Detailed balance is also not needed for a more general dynamics. We consider Markovian dynamics, with a master equation nonlinear in the distribution, P_n, as

$$\dot{P}_n \;=\; \sum_m \left[w_{nm}\, a(P_m) - w_{mn}\, a(P_n) \right]. \tag{12}$$

The stationarity condition defines

$$0 \;=\; \sum_m \left[w_{nm}\, a(Q_m) - w_{mn}\, a(Q_n) \right]. \tag{13}$$

The entropic distance formula is seeked in the trace form (but this time without the scaling assumption):

$$\rho[P,Q] \;=\; \sum_n \sigma(P_n, Q_n), \tag{14}$$

the dependence on Q_n is fixed by $\rho(Q,Q) = 0$. The change of the entropic divergence in this case is given by

$$\dot{\rho} \;=\; \sum_{m,n} \frac{\partial \sigma}{\partial P_n} \left[w_{nm}\, a(Q_m) \xi_m - w_{mn}\, a(Q_n) \xi_n \right] \tag{15}$$

with $\xi_n := a(P_n)/a(Q_n)$. We again put $\xi_m = \xi_n + (\xi_m - \xi_n)$ in the first summand:

$$\dot{\rho} \;=\; \sum_n \frac{\partial \sigma}{\partial P_n} \xi_n \cancel{\sum_m \left[w_{nm}\, a(Q_m) - w_{mn}\, a(Q_n) \right]} + \sum_{n,m} \frac{\partial \sigma}{\partial P_n} w_{nm}\, a(Q_m)\, (\xi_m - \xi_n) \tag{16}$$

In order to use the remainder theorem one has to identify

$$\frac{\partial \sigma}{\partial P_n} \;=\; \kappa'(\xi_n) \;=\; \kappa' \left(\frac{a(P_n)}{a(Q_n)} \right). \tag{17}$$

63 This ensures $\dot{\rho} < 0$ for any $\kappa'' > 0$ and $P \neq Q$.

We examine the example of the q–Kullback–Leibler or Rényi divergence. Starting with the classical logarithmic kernel, $\kappa(\xi) = -\ln \xi$, we have $\kappa''(\xi) = 1/\xi^2 > 0$. Now having a nonlinear stochastic dynamics, $a(P) = P^q$, the integrated entropic divergence formula (without symmetrization) delivers the Tsallis divergence [5–7],

$$\frac{\partial \sigma}{\partial P_n} \;=\; -\frac{Q_n^q}{P_n^q}, \qquad \Rightarrow \qquad \rho[P,Q] \;=\; \sum_n Q_n \ln_q \frac{Q_n}{P_n}. \tag{18}$$

with

$$\ln_q(x) = \frac{1 - x^{q-1}}{1-q} \tag{19}$$

64 being the so called deformed logarithm with the real parameter q.

We again would like to interpret this entropic divergence as entropy difference. The entropic divergence of the stationary distribution from the uniform distribution $U_n = 1/W, n = 1, 2, \ldots W$ is given by:

$$\rho[U,Q] \;=\; \sum_{n=1}^{W} \frac{Q_n}{1-q} \left[1 - (WQ_n)^{q-1} \right] \;=\; W^{q-1} \left(S_T[U] - S_T[Q] \right). \tag{20}$$

with S_T being the Tsallis entropy formula:

$$S_T[Q] \;=\; \frac{1}{1-q} \sum_n (Q_n^q - Q_n) \;=\; -\sum_n Q_n \ln_q(Q_n). \tag{21}$$

From the Jensen inequality it follows $\rho(U, Q) \geq 0$, so $S_T[U] \geq S_T[Q]$, i.e. the Tsallis entropy formula is also maximal for the uniform distribution. The factor W^{q-1} signifies non-extensivity, a dependence on the number of states in the relation between the entropic divergence and the relative Tsallis entropy.

4. Master equation for unidirectional growth and reset

With the particular choice of the transition rates, $w_{nm} = \mu_m \delta_{n-1,m} + \gamma_m \delta_{n,0}$, one describes a local growth process augmented with direct resetting transitions from any state to the ground state labelled by the index zero [8]. The corresponding master equation

$$\dot{P}_n \;=\; \mu_{n-1} P_{n-1} \;-\; (\mu_n + \gamma_n)\; P_n \tag{22}$$

is terminated at $n = 1$ and the equation for the $n = 0$ state takes care of the normalization conservation:

$$\dot{P}_0 \;=\; \sum_{n=1}^{\infty} \gamma_n P_n \;-\; \mu_0 P_0. \tag{23}$$

For the stationary distribution one obtains

$$Q_n \;=\; \frac{\mu_{n-1}}{\mu_n + \gamma_n}\, Q_{n-1} \;=\; \cdots \;=\; \frac{\mu_0 Q_0}{\mu_n} \prod_{j=1}^{n} \left(1 + \frac{\gamma_j}{\mu_j}\right)^{-1}, \tag{24}$$

and Q_0 has to be obtained from the normalization. Table 1 summarizes some well known probability density functions, PDF-s, which emerge as stationary distribution to this simplified stochastic dynamics upon different choices of the growth and reset rates μ_n and γ_n. In the continuous limit we obtain

$$\frac{\partial}{\partial t} P(x,t) \;=\; -\frac{\partial}{\partial x}\left(\mu(x)\, P(x,t)\right) - \gamma(x) P(x,t). \tag{25}$$

with the stationary distribution

$$Q(x) \;=\; \frac{K}{\mu(x)}\, \mathrm{e}^{-\int\limits_0^x \frac{\gamma(u)}{\mu(u)}\, du}. \tag{26}$$

Table 1. Summary of rates and stationary PDF-s.

$\gamma_n, \gamma(x)$	$\mu_n, \mu(x)$	$Q_n, Q(x)$
const	const	geometrical $\to$ exponential
const	linear	Waring $\to$ Tsallis/Pareto
const	sublinear power	Weibull
const	quadratic polynomial	Pearson
const	exp	Gompertz
$\ln(x/a)$	αx	Log-Normal
linear	const	Gauss
$\alpha(ax - c)$	αx	Gamma

Finally we derive a bound for the entropy production in the continuous model of unidirectional growth with resetting.

First we study the time evolution of the ratio, $\xi(t,x) = P(x,t)/Q(x)$. Using $P = \xi Q$ we get from eq.(25):

$$Q\,\frac{\partial \xi}{\partial t} \;=\; -\xi\, \cancel{\frac{\partial(\mu Q)}{\partial x}} - \mu Q\, \frac{\partial \xi}{\partial x} - \cancel{\gamma Q}\,\xi. \tag{27}$$

Using the same eq. for stationary $Q(x)$ and dividing by Q we obtain

$$\frac{\partial \xi}{\partial t} \; = \; -\mu(x)\, \frac{\partial \xi}{\partial x}. \tag{28}$$

Now we turn to the evolution of the entropic divergence,

$$\rho(t) \; \equiv \; \int\limits_0^{\infty} \mathfrak{s}(\xi(t,x))\, Q(x) dx, \tag{29}$$

With the symmetrized kernel, $\mathfrak{s}(\xi) = \sigma_{\text{div}}(\xi) + \xi\, \sigma_{\text{div}}(1/\xi) \geq 0$, one gets using $\dfrac{\partial \mathfrak{s}}{\partial t} = -\mu(x) \dfrac{\partial \mathfrak{s}}{\partial x}$ the following distance evolution, consiedring the boundary condition $\xi(t,0) = 1 \quad \text{and} \quad \mathfrak{s}(1) = 0$:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} \; = \; -\int\limits_0^{\infty} \mathfrak{s}(\xi(t,x))\, Q(x)\, \gamma(x) dx \tag{30}$$

We note that for the Kullback–Leibler divergence the following symmetrized kernel function has to be used: $\sigma(\xi) = -\ln \xi$ leads to $\mathfrak{s}(\xi) = (\xi - 1)\, \ln \xi$ and in this way ensures $\frac{\mathrm{d}\rho}{\mathrm{d}t} \leq 0$.

In order to obtain a lower bound for the speed of the approach to stationarity, we use again the Jensen inequalityfor $\mathfrak{s}(\xi)$:

$$\int p(x)\, \mathfrak{s}(\xi(x))\, dx \; \geq \; \mathfrak{s}\left(\int p(x)\, \xi(x)\, dx \right) \tag{31}$$

with any arbitrary $p(x) \geq 0$ satisfying $\int p(x)\, dx = 1$. For pour purpose we choose $p(x) = \gamma(x) Q(x) / \int \gamma Q\, dx$. This leads to the following result:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} \; \leq \; -\left\langle \gamma \right\rangle_{\infty} \cdot \mathfrak{s}\left(\frac{\left\langle \gamma \right\rangle_t}{\left\langle \gamma \right\rangle_{\infty}} \right) \; = \; \left[\left\langle \gamma \right\rangle_{\infty} - \left\langle \gamma \right\rangle_t \right] \cdot \ln \frac{\left\langle \gamma \right\rangle_t}{\left\langle \gamma \right\rangle_{\infty}}. \tag{32}$$

Note that the controlling quantity is actually the expectation value of the resetting rate, $\int p(x) \xi(x)\, dx = \int \gamma P\, dx = \left\langle \gamma \right\rangle_t$. Since $\mathfrak{s}(\xi)$ reaches its minimum with the value zero only at the argument 1, the entropic divergence $\rho(t)$ stops changing only if the stationary distribution is achieved. In all other cases it shrinks.

5. Summary

Summarizing in this paper we have presented a construction strategy for the entropic distance formula, designed to shrink for a given wide class of stochastic dynamics. The very entropy formula was then derived from inspecting this distance between the uniform distribution and the stationary PDF of the corresponding master equation. In this way for linear master equations the well-known Kullback–Leibler definition arises, while for nonlinear dependence on the occupation probabilities one always arrives at an accordingly modified expression. In particular for a general power-like dependence the Tsallis q-entropy occurs as the "natural" relative entropy interpretation of the proper entropic divergence. In the continuous version of the growth and reset master equation, a dissipative probability flow supported with an inflow at the boundary, a lower bound was given for the shrinking speed of the symmetrized entropic divergence using the Jensen inequality.

To finish this paper we would like to make some remarks on real world applications of the above discussed mathetmatical treatment. Among possible applications of the growth and resetting model we mention the network degree distributions showing exponential behavuior for constant rates and a Tsallis–Pareto distribution [9] (in the discrete version a Waring distribution [10,11]) for having a linear preference in the growth rate, $\mu_n = \alpha(n+b)$. For high energy particle abundance (hadron multiplicity) distributions the negative binomial PDF is an excellent approximation [12], when both rates μ and γ are linear functions of the state label. For middle and small settlement size distributions a log-normal PDF arise, achievable with linear growth rate, $\mu(x)$ and a logarithmic reset rate, $\gamma(x) \sim \ln x$. Citations of scientific papers and facebook shares and likes also follow a scaling Tsallis–Pareto distribution [13,14], characteristic to constant resetting and linear growth rates. While wealth seems to be distributed according to a Pareto-law tail, the middle class incomes rather show a gamma distribution, stemming from linear reset and growth rates. For a review of such applications see our forthcoming work.

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Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:
PDF – probability density function