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J. Stat. Mech. (2011) P06003

(http://iopscience.iop.org/1742-5468/2011/06/P06003)

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Measures of trajectory ensemble disparity in nonequilibrium statistical dynamics

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Received 15 April 2011
Accepted 12 May 2011
Published 3 June 2011

Online at stacks.iop.org/JSTAT/2011/P06003
doi:10.1088/1742-5468/2011/06/P06003

Abstract. Many interesting divergence measures between conjugate ensembles of nonequilibrium trajectories can be experimentally determined from the work distribution of the process. Herein, we review the statistical and physical significance of several of these measures, in particular the relative entropy (dissipation), Je reys divergence (hysteresis), Jensen–Shannon divergence (time-asymmetry), Cherno divergence (work cumulant generating function), and Rényi divergence.

Keywords: exact results, fluctuations (theory)

Contents

1. Csiszár f

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the same series of changes, in reverse, back to $\lambda(a)$. As a consequence of the time-reversal symmetry of the underlying dynamics, the ratio of the probability of a trajectory during the forward protocol $P[z|\Lambda]$ and the probability of its conjugate trajectory during the 11f 0..0036 Tc [-

For conjugate trajectory ensembles, the Je reys divergence is twice the hysteresis, the average dissipation of the forward and reverse protocols [26],

$$\begin{aligned}
\text{Je reys}(P[z|\Lambda]; P[\tilde{z}|\tilde{\Lambda}]) &= \beta\ W\ _{\Lambda} - \beta\Delta F_{\Lambda} + \beta\ W\ _{\tilde{\Lambda}} - \beta\Delta F_{\tilde{\Lambda}}, \\
&= \beta\ W\ _{\Lambda} + \beta\ W\ _{\tilde{\Lambda}} \\
&= 2 \times \text{hysteresis}. \qquad (10)
\end{aligned}$$

4. Jensen–Shannon divergence and time-asymmetry

The Jensen–Shannon divergence is defined as [30]

$$\begin{aligned}
\mathrm{JS}(p; q) &\equiv \tfrac{1}{2} D(p \quad \tfrac{1}{2}(p + q)) + \tfrac{1}{2} D(q \quad \tfrac{1}{2}(p + q)) \\
&= \frac{1}{2} \sum_{i}
\end{aligned}$$

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The Jensen–Shannon and Je reys divergences are related by the inequalities [5, 26]

$$\mathrm{JS}(p;q) \leq \tfrac{1}{8}\mathrm{Je\ \ reys}(p;q) \qquad \mathrm{JS}(p;q) \leq \ln \frac{2}{1 + \exp(-(1/2)\mathrm{Je\ \ reys}(p;q))}. \tag{14}$$

These inequalities imply that a given time-asymmetry requires a certain minimum hysteresis.

5. Cherno divergence and work cumulant generating functions

The Cherno divergence of order α is defined as [33, 34]

$$\begin{aligned} \mathrm{Cherno}\ \ _{\alpha}(p;q) &\equiv -\ln \sum_i p_i \left(\frac{p_i}{q_i}\right)^{\alpha-1}, \\ &= -\ln[C_f(p;q) + 1], \qquad f(x) = x^{1-\alpha} - 1. \end{aligned} \tag{15}$$

The Cherno divergence is zero for $\alpha = 1$ and 0, and reaches a maximum, the Cherno information [22, 33], for some intermediate value of α. The Cherno divergence is well defined for $\alpha > 1$ if $q_i > 0$ whenever $p_i > 0$, and for $\alpha < 0$ if $p_i > 0$ whenever $q_i > 0$, and thus defined for all α if the distributions have the same support.

The Cherno divergence of order α is related to the Cherno divergence of order $1-\alpha$ with the distributions interchanged [34],

$$\mathrm{Cherno}\ \ _{\alpha}(p;q) = \mathrm{Cherno}\ \ _{1-\alpha}(q;p). \tag{16}$$

This relation always holds for α [0, 1], and for all α when the distributions have the same support.

For conjugate trajectory ensembles, the Cherno divergence of order $1 - \alpha$ is proportional to the cumulant generating function for the excess work,

$$\mathrm{Cherno}\ \ _{1-\alpha}(P[z|\Lambda]; P[\tilde{z}|\tilde{\Lambda}]) = -\ln\ \mathrm{e}^{-\alpha(\beta W - \beta\Delta F)}\ \ _{\Lambda}. \tag{17}$$

Recall that a cumulant generating function has the form

$$\ln\ \mathrm{e}\ \ = \sum_{=1}^{\infty} t$$

or equivalently

$$\ln \ \mathrm{e}^{-\alpha\beta W} \ _{\Lambda} = \ln \ \mathrm{e}^{-(1-\alpha)\beta W} \ _{\tilde{\Lambda}} - \beta \Delta F_{\Lambda}. \tag{21}$$

Note that an additional minus sign enters into the right hand expression because both the work and free energy change are odd under time-reversal, $W[z, \Lambda] - \Delta F_{\Lambda} = -W[\tilde{z}, \tilde{\Lambda}] + \Delta F_{\tilde{\Lambda}}$. If we set $\alpha = 1$ or 0 we recover the Jarzynski identity, $\ln \ \exp\{-\beta W\} \ _{\Lambda} = -\beta \Delta F_{\Lambda}$ [16].

This symmetry between cumulant generating functions implies that the work cumulants under a given protocol are related to the work cumulants of the conjugate protocol [36],

$$\kappa \ [\beta W|\Lambda] = \sum_{=}^{\infty} \frac{(-1)}{(n-k)!} \kappa \ [\beta W|\tilde{\Lambda}]. \tag{22}$$

From this relation Hummer and Szabo [36, 37] derive optimal estimators of free energy, given only the first m work cumulants. In a parallel development, this symmetry is also exploited in the large deviation approach to steady state fluctuation theorems [35].

The case $\alpha = \frac{1}{2}$ is related to the Bhattacharyya distance, another measure of probability distribution overlap [38],

$$\begin{aligned} \mathrm{Bhattacharyya}(p; q) &= -\ln \sum_{i} \sqrt{p_i q_i} \\ &= \mathrm{Cherno} \ _{\frac{1}{2}}(p; q). \end{aligned} \tag{23}$$

The Bhattacharyya distance is invariant to interchange of p and q

7. Illustrative analytic example

To make these relations more concrete, we consider a system consisting of a micron-sized bead suspended in water at inverse temperature β by an initially stationary optical laser trap, with spring constant k. The trap is then translated at a constant velocity v, dragging the bead through the fluid with friction coefficient γ for a time t. This system can be modeled by a single particle undergoing overdamped Langevin dynamics in a one dimensional moving harmonic potential, and the pertinent properties of the model have been analyzed [27, 41]. The free energy change is zero and the work distribution is Gaussian with mean

$$W_0 \equiv \gamma v^2 [t - (1 - e^{-\;/\gamma})\,\gamma/k], \tag{31}$$

and variance $2W_0$.

The relative entropy, Jeffreys divergence and Chernoff divergence for this model are all simple functions of βW_0:

$$\begin{aligned} &D(P[z|\Lambda]\,\|\,P[\tilde{z}|\tilde{\Lambda}]) = \beta W_0, \qquad \text{Jeffreys}(P[z|\Lambda];P[\tilde{z}|\tilde{\Lambda}]) = 2\beta W_0, \\ &\text{Chernoff}_{1-\alpha}(P[z|\Lambda];P[\tilde{z}|\tilde{\Lambda}]) = \alpha(\alpha-1)\beta W_0. \end{aligned} \tag{32}$$

The Jensen–Shannon divergence does not appear to have a simple closed-form solution for this system.

8. Epilogue

As we have seen, a number of f-divergences have both interesting statistical and physical interpretations for conjugate ensembles of nonequilibrium trajectories, and can be measured in computer simulation and real world experiments. This allows us to exploit