The Maximum Caliber principle applied to continuous systems

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Abstract. We give a brief presentation of the maximization of path entropy (Maximum Caliber) formalism as an approach to inference over trajectories. We develop its continuous–time version involving path integrals and present an identity between expectations over the most unbiased probability distribution of trajectories. This relation between expectations can be used to solve for the Lagrange multipliers in a Maximum Caliber problem without the need for the dynamical partition function.

1. Introduction

Although theoretically equilibrium is the fundamental concept in Thermodynamics, in practice most systems studied in a laboratory are systems out of equilibrium. This closeness to reality is what gives tremendous importance to the development of a formalism for describing these systems. Finding a formalism based on as few as possible principles and consistent with the principle of maximum entropy [1] in the case of equilibrium, which is still valid for a time-dependent treatment of statistical properties of a system, is the goal of much ongoing research. A proposal which has recently gained visibility in the statistical physics community is the principle of maximum path entropy or maximum *caliber* [2, 3].

In this framework, a probability functional associates a probability to every possible path the system can take when going from point A to point B. This probability functional can be directly used to predict expectations of functional properties and also instantaneous properties (through a *time-slicing* procedure), in what promises to become a useful tool for non-equilibrium systems. It is also expected that the non-equilibrium formalism by Evans *et al* [4] can be recovered from this single principle.

2. The Maximum Caliber principle

In the same way that the principle of Maximum Entropy (MaxEnt for short) produces the most unbiased probability distribution consistent with some constraint $\left\langle f(\vec{x}) \right\rangle = F$ by maximizing the Gibbs-Shannon entropy functional

$$S[p] = - \int d\vec{x}\, p(\vec{x}) \ln p(\vec{x}) \tag{1}$$

under said constraints, the principle of Maximum Caliber (MaxCal) replaces the microstates $\vec{x}$ with micro-trajectories $x(t)$. Then, the functional corresponding to the Gibbs-Shannon entropy is called the *caliber*,

$$C[p] = -\int Dx() p[x()] \ln p[x()] \tag{2}$$

where the integral is now a functional integral over all trajectories (denoted by $Dx()$) and $p[x()]$ is a probability functional.

When the caliber in Eq. 2 is maximized under the constraints of normalization,

$$\int Dx() P[x()] = \Big\langle 1 \Big\rangle = 1, \tag{3}$$

and a known expectation of a functional

$$\Big\langle F[x()] \Big\rangle = \int Dx() P[x()] F[x()] = F_0, \tag{4}$$

the most unbiased distribution of trajectories is of the form

$$P[x()] = \frac{1}{Z} \exp(-\lambda F[x()]), \tag{5}$$

with Z a normalization constant, given by

$$Z = \int Dx() \exp(-\lambda F[x()]). \tag{6}$$

The Lagrange multiplier λ can be obtained, as in MaxEnt, from

$$-\frac{\partial}{\partial \lambda} \ln Z(\lambda) = F_0. \tag{7}$$

Equivalently, if an instantaneous property is known in expectation for each time t in an interval, $t \in [0, T]$,

$$\Big\langle G(x(t), \dot{x}(t), t) \Big\rangle = \int Dx() P[x()] G[x(); t] = g(t) \tag{8}$$

the probability functional is of the form

$$P[x()] = \frac{1}{\eta} \exp\left(-\int_0^T dt \lambda(t) G(x(t), \dot{x}(t); t)\right). \tag{9}$$

This is equivalent to the first kind of constraint (Eq. 4), because clearly if we integrate Eq. 8 in t from 0 to T we see that we are constraining the expectation of a *functional*

$$F[x()] = \int_0^T dt \lambda(t) G(x(t), \dot{x}(t); t), \tag{10}$$

in the sense of Eq. 4.

In the case of constraints as expressed in Eq. 8, the Lagrange multiplier function can be obtained, in an analogous way to Eq. 7, from

$$-\frac{\delta}{\delta \lambda(t)} \ln Z[\lambda()] = g(t). \tag{11}$$

If the instantaneous property G depends only on the instantaneous position $x(t)$ and velocity $\dot{x}(t)$ (and possible, explicitly on time), the functional F has the form of the classical action $A[x()]$ in mechanics

$$A[x()] = \int_0^T dt \mathcal{L}(x(t), \dot{x}(t); t), \tag{12}$$

and, in fact, if $\lambda > 0$ the most probable trajectory is the one which minimizes $A[x()]$, i.e., the principle of minimum action [5].

3. Conjugate variables theorem (CVT) for functionals

Once given the form of the probability functional (Eq. 5), we look for analytical tools that allows us to evaluate expectations of different properties. In MaxEnt there is such an identity, known as the conjugate variables theorem (CVT) [6], itself a direct consequence of the divergence theorem.

For an arbitrary distribution $p(\vec{x})$, we have

$$\left\langle \nabla \cdot \vec{v}(\vec{x}) \right\rangle + \left\langle \vec{v}(\vec{x}) \cdot \nabla \ln p \right\rangle = 0. \tag{13}$$

where the expectations are taken under the distribution p, and $\vec{v}(\vec{x})$ is an arbitrary (differentiable) vector field. We look for a generalization for MaxCal, i.e., when $\vec{x} \to x(t)$.

Consider the functional derivative of a product of functionals,

$$\frac{\delta}{\delta x(t)}\Big(P[x()]G[x()]\Big) = \frac{\delta P[x()]}{\delta x(t)}G[x()] + \frac{\delta G[x()]}{\delta x(t)}P[x()]. \tag{14}$$

If we rewrite the functional derivative of $P[x()]$ as

$$\frac{\delta P[x()]}{\delta x(t)} = P[x()]\frac{\delta}{\delta x(t)}\ln P[x()], \tag{15}$$

and replace in Eq. 14, we get

$$\frac{\delta}{\delta x(t)}\Big(P[x()]G[x()]\Big) = P[x()]\left[G[x()]\frac{\delta}{\delta x(t)}\ln P[x()] + \frac{\delta G[x()]}{\delta x(t)}\right]. \tag{16}$$

Now we integrate over all trajectories $x()$,

$$\int Dx()\frac{\delta}{\delta x(t)}\Big(P[x()]G[x()]\Big) = \int Dx()P[x()]G[x()]\frac{\delta}{\delta x(t)}\ln P[x()] + \int Dx()P[x()]\frac{\delta G[x()]}{\delta x(t)}, \tag{17}$$

and, as the probability functional P can be normalized, the "surface integral" on the left hand side vanishes. Therefore, we arrive at the following identity, generalization of Eq. 13 for functionals,

$$\left\langle \frac{\delta G[x()]}{\delta x(t)} \right\rangle + \left\langle G[x()]\frac{\delta}{\delta x(t)}\ln P[x()] \right\rangle = 0, \tag{18}$$

where $G[x()]$ corresponds to an arbitrary functional. For a Maximum Caliber probability functional (Eq. 5), this reduces to

$$\left\langle \frac{\delta G[x()]}{\delta x(t)} \right\rangle = \lambda \left\langle G[x()]\frac{\delta}{\delta x(t)}F[x()] \right\rangle. \tag{19}$$

This means we can avoid Eq. 7 to solve for λ, simply obtaining it from

$$\lambda = \frac{\left\langle \frac{\delta}{\delta x(t)}G[x()] \right\rangle}{\left\langle G[x()]\frac{\delta}{\delta x(t)}F[x()] \right\rangle}. \tag{20}$$

Using Eq. 19 with a constant functional, $G[x()] = 1$, we see that

$$\left\langle \frac{\delta}{\delta x(t)} F[x()] \right\rangle = \left\langle \frac{\delta}{\delta x(t)} A[x()] \right\rangle = 0, \tag{21}$$

that is, the principle of minimum action also holds in expectation. A particular case of this relation is the result in Ref. [5],

$$\left\langle \dot{p}(t) \right\rangle = -\left\langle \Phi'(x(t)) \right\rangle, \tag{22}$$

which is the expectation of Newton's second law.

4. Conclusions
We have shown that the Maximum Caliber principle is a powerful tool to study dynamical systems in a probabilistic framework. A generalization of the conjugate variables theorem (CVT) is presented for probability functionals, from which we prove that the minimum action principle holds also in expectation over the ensemble of trajectories. This "functional CVT" can also be used to find novel relations between expectations of functionals.

Acknowledgments

References
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