A Noether Theorem for Markov Processes

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Abstract

Noether's theorem links the symmetries of a quantum system with its conserved quantities, and is a cornerstone of quantum mechanics. Here we prove a version of Noether's theorem for Markov processes. In quantum mechanics, an observable commutes with the Hamiltonian if and only if its expected value remains constant in time for every state. For Markov processes that no longer holds, but an observable commutes with the Hamiltonian if and only if both its expected value and standard deviation are constant in time for every state.

1 Introduction

There is a rich analogy between quantum mechanics and what one might call 'stochastic mechanics', where probabilities take the place of amplitudes [1]. In quantum mechanics, we specify the state of a system by an element ψ of a Hilbert space, and describe its time evolution by the Schrödinger equation:

$$\frac{d}{dt}\psi = -iH\psi$$

where H is a self-adjoint linear operator called the Hamiltonian. For Markov processes, we specify the state of a system by a probability distribution ψ on some measure space, and describe its time evolution by the so-called 'master equation'

$$\frac{d}{dt}\psi = H\psi$$

where H is a linear operator variously known as a 'stochastic Hamiltonian', 'transition rate matrix' or 'intensity matrix'. In quantum mechanics, it is well-known that conserved quantities correspond to self-adjoint operators that commute with the Hamiltonian. Here we present a similar result for Markov processes.

To avoid technicalities and focus on the basic idea, we start by considering Markov processes, or technically 'Markov semigroups', where the measure space X is just a finite set equipped with its counting measure. Later we consider the general case. We begin by reviewing some basic facts and setting up some definitions; for details see Stroock [7].

When X is a finite set, a **probability distribution** on X is a function $\psi: X \to \mathbb{R}$ such that $\psi_i \geq 0$ for all $i \in X$ and

$$\sum_{i \in X} \psi_i = 1$$

We say an operator $U: \mathbb{R}^X \to \mathbb{R}^X$ is **stochastic** if it is linear and it maps probability distributions to probability distributions. A **Markov semigroup** consists of operators $U(t): \mathbb{R}^X \to \mathbb{R}^X$, one for each $t \in [0, \infty)$, such that:

- (i) U(t) is stochastic for all $t \ge 0$.
- (ii) U(t) depends continuously on t.
- (iii) U(s+t) = U(s)U(t) for all $s, t \ge 0$.
- (iv) U(0) = I.

Any Markov semigroup may be written as $U(t) = \exp(tH)$ for a unique linear operator $H : \mathbb{R}^X \to \mathbb{R}^X$. Moreover, this operator H is **infinitesimal stochastic**, meaning that if we write it as a matrix using the canonical basis for \mathbb{R}^X , then:

- (i) $H_{ij} \ge 0$ for all $i, j \in X$ with $i \ne j$.
- (ii) $\sum_{i \in X} H_{ij} = 0$ for all $j \in X$.

For $i \neq j$ the matrix entry H_{ij} is the probability per time of a transition from the state $j \in X$ to the state $i \in X$. Condition (i) says that these probabilities are nonnegative. Condition (ii) then says that the diagonal entry H_{ii} is minus the probability per time of a transition out of the state i.

Conversely, for any infinitesimal stochastic operator $H \colon \mathbb{R}^X \to \mathbb{R}^X$, $\exp(tH)$ is a Markov semigroup. Given any function $\psi \colon X \to \mathbb{R}$, we obtain a solution for $t \in [0, \infty)$ of the **master equation**:

$$\frac{d}{dt}\psi(t) = H\psi(t)$$

with H as **Hamiltonian** and ψ as the initial value by setting

$$\psi(t) = \exp(tH)\psi.$$

If ψ is a probability distribution, then so is $\psi(t)$ for all $t \ge 0$.

Next we turn to Noether's theorem. There are many theorems of this general type, all of which relate symmetries of a physical system to its conserved quantities. Noether's original version applies to the Lagrangian approach to classical mechanics, and obtains conserved quantities from symmetries of the Lagrangian [3, 5]. This version has been generalized to stochastic mechanics by a number of authors [2, 6, 8]. In the Hamiltonian approach to classical mechanics, any observable having vanishing Poisson bracket with the Hamiltonian both generates symmetries of the Hamiltonian and is a conserved quantity. This idea extends to quantum mechanics if we replace Poisson brackets by commutators. It is this last form of Noether's theorem, somewhat removed from the original form but very easy to prove, that we now generalize to Markov processes. For a Markov process, an observable will commute with the Hamiltonian if and only if both its expected value and that of its square are constant in time for every state.

Here an **observable** is a function $O: X \to \mathbb{R}$ assigning a real number O_i to each state $i \in X$. We identify O with the diagonal matrix with *ii*th entry equal to O_i , and define its **expected value** for a probability distribution ψ to be

$$\langle O, \psi \rangle = \sum_{i \in X} O_i \psi_i.$$

Our Noether theorem for finite Markov processes may then be stated as follows:

Proposition (Noether's Theorem, Stochastic Version). Let X be a finite set, let $H: \mathbb{R}^X \to \mathbb{R}^X$ be an infinitesimal stochastic operator, and let O be an observable. Then [O, H] = 0 if and only if for all families of probability distributions $\{\psi(t) \mid t \in [0, \infty)\}$ obeying the master equation $\frac{d}{dt}\psi(t) = H\psi(t)$, the expected values $\langle O, \psi(t) \rangle$ and $\langle O^2, \psi(t) \rangle$ are constant.

For comparison, in the quantum version, both the Hamiltonian and the observable are given by self-adjoint operators on a Hilbert space. To avoid technicalities, we only state the version for bounded operators:

Proposition (Noether's Theorem, Quantum Version). Let H and O be bounded self-adjoint operators on a Hilbert space. Then [O, H] = 0 if and only if for all families of states $\{\psi(t) \mid t \in [0, \infty)\}$ obeying Schrödinger's equation $\frac{d}{dt}\psi(t) = -iH\psi(t)$, the expected value $\langle \psi(t), O\psi(t) \rangle$ is constant.

The similarity between these two results is striking, but this also illuminates a key difference: the Markov version requires not just the expected value of the observable to be constant, but also the expected value of its square. This condition cannot be weakened to only require that the expected value be constant. Observe that if

$$H = \begin{pmatrix} 0 & 1 & 0 \\ 0 & -2 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad O = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

then for the initial value $\psi = (0, 1, 0)$, we have $\frac{d}{dt} \langle O, \psi(t) \rangle = 0$ for all $t \ge 0$, but $[O, H] \ne 0$.

Indeed, in both the quantum and stochastic cases, the time derivative of the expected value of an observable O is expressed in terms of the commutator [O, H]. In the quantum case we have

$$\frac{d}{dt}\langle\psi(t),O\psi(t)\rangle = -i\langle\psi(t),[O,H]\psi(t)\rangle$$

for any solution $\psi(t)$ of Schrödinger's equation. The polarisation identity then implies that the right-hand side vanishes for all solutions if and only if [O, H] = 0. In the stochastic case we have

$$\frac{d}{dt}\langle O,\psi(t)\rangle = \langle 1, [O,H]\psi(t)\rangle$$

for any solution $\psi(t)$ of the master equation. However, in this case the right-hand side can vanish for all solutions $\psi(t)$ without [O, H] = 0, as shown by the above example. To ensure [O, H] = 0 we need a supplementary hypothesis, such as the vanishing of $\frac{d}{dt} \langle O^2, \psi(t) \rangle$.

What is the meaning of this supplementary hypothesis? Including it means that not only is the expected value of the observable O conserved, but so is its **variance**, defined by

$$\langle O^2, \psi \rangle - \langle O, \psi \rangle^2$$

Of course the variance is the square of the standard deviation of O, so an observable commutes with the Hamiltonian if and only if both its expected value and standard deviation are constant in time for every state.

2 A Noether theorem for finite Markov processes

While proving Noether's theorem for finite Markov processes it is enlightening to introduce some other equivalent characterizations of conserved quantities. For this we shall introduce the **transition** graph of an infinitesimal stochastic operator. Suppose X is a finite set and $H: \mathbb{R}^X \to \mathbb{R}^X$ is an infinitesimal stochastic operator. We may form a directed graph with the set X as vertices and an edge from j to i if and only if $H_{ij} \neq 0$. We say i and j are in the same **connected component** of this graph if there is a sequence of vertices $j = k_0, k_1, \ldots, k_n = i$ such that for each $0 \leq \ell < n$ there is either an edge from k_ℓ to $k_{\ell+1}$ or from $k_{\ell+1}$ to k_ℓ .

Our Noether theorem is the equivalence of (i) and (iii) in the following theorem:

Theorem 1. Let X be a finite set, let $H: \mathbb{R}^X \to \mathbb{R}^X$ be an infinitesimal stochastic operator, and let O be an observable. Then the following are equivalent:

- (*i*) [O, H] = 0.
- (ii) $\frac{d}{dt}\langle f(O), \psi(t) \rangle = 0$ for all polynomials $f \colon \mathbb{R} \to \mathbb{R}$ and all ψ satisfying the master equation with Hamiltonian H.
- (iii) $\frac{d}{dt}\langle O, \psi(t) \rangle = \frac{d}{dt}\langle O^2, \psi(t) \rangle = 0$ for all ψ satisfying the master equation with Hamtiltonian H.
- (iv) $O_i = O_j$ if i and j lie in the same connected component of the transition graph of H.

Proof. We prove (i) \Rightarrow (ii) \Rightarrow (iii) \Rightarrow (iv) \Rightarrow (i).

(i) \Rightarrow (ii) As *H* commutes with *O*, *H* commutes with f(O) whenever *f* is a polynomial. From this and the master equation we have

$$\frac{d}{dt}\langle f(O),\psi(t)\rangle = \langle f(O),\frac{d}{dt}\psi(t)\rangle = \langle f(O),H\psi(t)\rangle = \langle 1,f(O)H\psi(t)\rangle = \langle 1,Hf(O)\psi(t)\rangle$$

But H is infinitesimal stochastic, so

$$\langle 1, Hf(O)\psi(t)\rangle = \sum_{i,j\in X} H_{ij}f(O_j)\psi_j(t) = \sum_{j\in X} \left(\sum_{i\in X} H_{ij}\right)f(O_j)\psi_j(t) = 0.$$

(ii) \Rightarrow (iii) Both O and O^2 are polynomials in O.

(iii) \Rightarrow (iv) Suppose that $i, j \in X$ lie in the same connected component. We claim that then $O_i = O_j$. As equality is transitive, it suffices to show $O_i = O_j$ whenever $H_{ij} \neq 0$. For this it suffices to show that for any $j \in X$ we have

$$\sum_{i \in X} (O_j - O_i)^2 H_{ij} = 0.$$

This is enough, as each term in this sum is nonnegative: when i = j we have $O_j - O_i = 0$, while when $i \neq j$, both $(O_j - O_i)^2$ and H_{ij} are nonnegative—the latter because H is infinitesimal stochastic. Thus when their sum is zero each term $(O_j - O_i)^2 H_{ij}$ is zero. But this means that if H_{ij} is nonzero, then $O_i = O_j$, and this proves the claim.

Expanding the above expression then, we have

$$\sum_{i \in X} (O_j - O_i)^2 H_{ij} = O_j^2 \sum_{i \in X} H_{ij} - 2O_j \sum_{i \in X} O_i H_{ij} + \sum_{i \in X} O_i^2 H_{ij}.$$

The three terms here are each zero: the first because H is infinitesimal stochastic, and the latter two since, if e_j is the probability distribution with value 1 at $j \in X$ and 0 elsewhere, then

$$\left. \frac{d}{dt} \langle O, \exp(tH)e_j \rangle \right|_{t=0} = \langle O, He_j \rangle = \sum_{i \in X} O_i H_{ij}$$

and

$$\left. \frac{d}{dt} \langle O^2, \exp(tH) e_j \rangle \right|_{t=0} = \langle O^2, H e_j \rangle = \sum_{i \in X} O_i^2 H_{ij},$$

and by hypothesis these two derivatives are both zero.

(iv) \Rightarrow (i) When H_{ij} is nonzero, the states *i* and *j* lie in the same component, so $O_i = O_j$. Thus for each $i, j \in X$:

$$[O,H]_{ij} = (OH - HO)_{ij} = O_i H_{ij} - H_{ij} O_j = (O_i - O_j) H_{ij} = 0.$$

3 A Noether theorem for general Markov processes

In this section we generalize Noether's theorem for Markov processes from the case of a finite set of states to a more general measure space. This seems to require some new ideas and techniques.

Suppose that X is a σ -finite measure space with a measure we write simply as dx. Then probability distributions ψ on X lie in $L^1(X)$. We define an **observable** O to be any element of the dual Banach space $L^{\infty}(X)$, allowing us to define the expected valued of O in the probability distribution ψ to be

$$\langle O, \psi \rangle = \int_X O(x)\psi(x) \, dx.$$

We can also think of an observable O as a bounded operator on $L^1(X)$, namely the operator of multiplying by the function O.

Let us say that an operator $U: L^1(X) \to L^1(X)$ is **stochastic** if it is linear, bounded, and maps probability distributions to probability distributions. Equivalently, U is stochastic if it is linear and obeys

$$\psi \ge 0 \implies U\psi \ge 0$$

and

$$\int_{X} (U\psi)(x) \, dx = \int_{X} \psi(x) \, dx$$

for all $\psi \in L^1(X)$. We may also write the latter equation as

$$\langle 1, U\psi \rangle = \langle 1, \psi \rangle.$$

A Markov semigroup is a strongly continuous one-parameter semigroup of stochastic operators $U(t): L^1(X) \to L^1(X)$. By the Hille–Yosida theorem [9], any Markov semigroup may be written as $U(t) = \exp(tH)$ for a unique closed operator H on $L^1(X)$. Any operator H that arises in this way is infinitesimal stochastic. However, such operators are typically unbounded and only densely defined. This makes it difficult to work with the commutator [O, H], because the operator O may not preserve the domain of H. From our experience with quantum mechanics, the solution is to work instead with the commutators $[O, \exp(tH)]$, which are bounded operators defined on all of $L^1(X)$. This amounts to working directly with the Markov semigroup instead of the infinitesimal stochastic operator H.

Theorem 2. Suppose X is a σ -finite measure space and

$$U(t): L^1(X) \to L^1(X)$$

is a Markov semigroup. Suppose O is an observable. Then [O, U(t)] = 0 for all $t \ge 0$ if and only if for all probability distributions ψ on X, the expected values $\langle O, U(t)\psi \rangle$ and $\langle O^2, U(t)\psi \rangle$ are constant as a function of t.

This result is an easy consequence of the following one, which is of interest in its own right, since it amounts to a Noether's theorem for Markov chains. A 'Markov chain' is similar to a Markov process, but time comes in discrete steps, and at each step the probability distribution ψ evolves via $\psi \mapsto U\psi$ for some stochastic operator U.

Theorem 3. Suppose X is a σ -finite measure space and $U: L^1(X) \to L^1(X)$ is a stochastic operator. Suppose O is an observable. Then [O, U] = 0 if and only if for all probability distributions ψ on X, $\langle O, U\psi \rangle = \langle O, \psi \rangle$ and $\langle O^2, U\psi \rangle = \langle O^2, \psi \rangle$. *Proof.* First, suppose [O, U] = 0. Note

$$\langle O, \phi \rangle = \langle 1, O\phi \rangle$$

and since U is stochastic, also

$$\langle 1, U\phi \rangle = \langle 1, \phi \rangle$$

for all $\phi \in L^1(X)$. Thus, for any probability distribution ψ on X and any $n \ge 0$ we have

$$\langle O^n, U\psi \rangle = \langle 1, O^n U\psi \rangle = \langle 1, UO^n \psi \rangle = \langle 1, O^n \psi \rangle = \langle O^n, \psi \rangle$$

Taking n = 1, 2 we get the desired result.

To prove the converse, we use three lemmas. In all these X is a σ -finite measure space, $U: L^1(X) \to L^1(X)$ is a stochastic operator, and O is an observable. We freely switch between thinking of O as a function in $L^{\infty}(X)$ and the operator on $L^1(X)$ given by multiplying by that function.

Lemma 1. Suppose that for any compact interval $I \subseteq \mathbb{R}$ the operator U commutes with $\chi_I(O)$, meaning the operator on $L^1(X)$ given by multiplying by the characteristic function of

$$O^{-1}(I) = \{ x \in X : O(x) \in I \}.$$

Then U commutes with O.

Proof. The range of the function O is contained in the interior of some interval [-M, M]. The step functions

$$f_n = \sum_{i=-n}^{n-1} \frac{iM}{n} \chi_{\left[\frac{iM}{n}, \frac{(i+1)M}{n}\right]}$$

are uniformly bounded and converge pointwise to the identity function on the range of O, so by the dominated convergence theorem $f_n(O)\psi \to O\psi$ in the L^1 norm for all $\psi \in L^1(X)$. Furthermore, though we have not written it as such, f_n is a linear combination of characteristic functions of compact intervals, since we include a single point as a degenerate special case of a compact interval. Thus, by hypothesis, U commutes with $f_n(O)$. It follows that for every $\psi \in L^1(X)$, we have

$$OU\psi = \lim_{n \to \infty} f_n(O)U\psi$$

=
$$\lim_{n \to \infty} Uf_n(O)\psi$$

=
$$UO\psi.$$

Lemma 2. Suppose that for every compact interval I and every $\psi \in L^1(X)$,

$$\operatorname{supp}(\psi) \subseteq O^{-1}(I) \implies \operatorname{supp}(U\psi) \subseteq O^{-1}(I).$$

Then U commutes with every operator $\chi_I(O)$.

Proof. The set of L^1 functions supported in $O^{-1}(I)$ is the range of the operator $\chi_I(O)$, so the hypothesis says that U maps the range of this operator to itself. Given any $\psi \in L^1(X)$ and writing $p = \chi_I(O)$, we have

$$\psi = p\psi + (1-p)\psi$$

 \mathbf{SO}

$$pU\psi = pUp\psi + pU(1-p)\psi.$$

Since U preserves the range of p and p is the identity on this range, we have $pUp\psi = Up\psi$. Since the range of the function O is contained in some interval [-M, M], we can write 1 - p as a linear combination of operators $\chi_J(O)$ for other compact intervals J, again using the fact that a point is a degenerate case of a compact interval. Thus U also preserves the range of 1 - p. Since the range of 1 - p is the kernel of p, $pU(1 - p)\psi = 0$. We thus have

$$pU\psi = Up\psi.$$

Lemma 3. Suppose that $\langle O, U\psi \rangle = \langle O, \psi \rangle$ and $\langle O^2, U\psi \rangle = \langle O^2, \psi \rangle$ for all $\psi \in L^1(X)$. Then for every compact interval I and every $\psi \in L^1(X)$,

$$\operatorname{supp}(\psi) \subseteq O^{-1}(I) \implies \operatorname{supp}(U\psi) \subseteq O^{-1}(I)$$

Proof. The range of O is contained in the interior of some interval [-M, M]. Thus we shall only prove the lemma for I contained in (-M, M), since otherwise we can replace I by a smaller compact interval with this property without changing $O^{-1}(I)$.

Suppose ψ is supported in $O^{-1}(I)$. We wish to show the same for $U\psi$. It suffices to show that $U\psi$ is supported in $O^{-1}(J)$ where J is any compact interval with $I \subseteq int(J) \subseteq (-M, M)$. Moreover, we may assume that ψ is a probability distribution, since any L^1 function supported in $O^{-1}(I)$ is a linear combination of two probability distributions supported in this set.

To show that $U\psi$ is supported in $O^{-1}(J)$, we write

$$\psi = \sum_{i=-n}^{n-1} \psi_i$$

where

$$\psi_i = \chi_{\left[\frac{iM}{n}, \frac{(i+1)M}{n}\right)}(O) \,\psi.$$

We thus have

$$U\psi = \sum_{i=-n}^{n-1} U\psi_i.$$

We shall show that

$$\|(1 - \chi_J(O))U\psi_i\|_1 \le \frac{c}{n^2} \,\|\psi_i\|_1 \tag{1}$$

for some constant c. It follows that

$$\|(1-\chi_J(O))U\psi\|_1 \le \sum_{i=-n}^{n-1} \|(1-\chi_J(O))U\psi_i\|_1 \le \frac{c}{n^2} \sum_{i=-n}^{n-1} \|\psi_i\|_1 = \frac{c}{n^2} \|\psi\|_1 = \frac{c}{n^2}$$

for all n, and thus

$$\|(1 - \chi_J(O))U\psi\|_1 = 0$$

so $U\psi$ is supported in $O^{-1}(J)$.

To prove (1) we shall use Chebyshev's inequality, which says that the probability of a random variable taking a value at least k standard deviations away from its mean is less than or equal to $1/k^2$. However, we first need to convert probability functions on X into probability measures on the real line.

For any function $\psi \in L^1(X)$ we can push forward the signed measure $\psi \, dx$ on X via $O: X \to \mathbb{R}$ to obtain a signed measure on \mathbb{R} , which we call $\tilde{\psi}$. Concretely, $\tilde{\psi}$ is characterized by the equation

$$\int_{X} f(O(x))\psi(x) \, dx = \int_{\mathbb{R}} f \, \widetilde{\psi}$$

which holds for any bounded measurable function $f \colon \mathbb{R} \to \mathbb{R}$. Since the integral at left only depends on the value of f in the interval [-M, M], the same is true for the integral at right, so with no harm we can restrict f and the integral to [-M, M]. Clearly

$$\widetilde{(\phi + \chi)} = \widetilde{\phi} + \widetilde{\chi}$$
$$\widetilde{(\alpha \phi)} = \alpha \, \widetilde{\phi}$$

and

for all $\alpha \in \mathbb{R}$ and $\phi, \chi \in L^1(X)$. If ϕ is nonnegative then ϕ is a nonnegative measure, and if ϕ is a probability distribution then ϕ is a probability measure.

Since we are assuming that the function ψ is supported in $O^{-1}I$, the measure $\tilde{\psi}$ is supported in I. Since

$$\psi_i = \chi_{\left[\frac{iM}{n}, \frac{(i+1)M}{n}\right)}(O)\psi$$

we have

$$\widetilde{\psi}_i = \chi_{\left[\frac{iM}{n}, \frac{(i+1)M}{n}\right)} \, \widetilde{\psi}.$$

In what follows we assume ψ_i is nonzero, since otherwise (1) is trivial. This implies that we can rescale $\tilde{\psi}_i$ to obtain a probability measure, namely

$$\frac{1}{\|\psi_i\|_1}\,\widetilde{\psi}_i$$

Since this probability measure is supported in the interval $I \cap [iM/n, (i+1)M/n)$, clearly its mean lies in I, and its standard deviation is less than M/n.

By our hypotheses on U,

$$\frac{1}{\|\psi_i\|_1}\widetilde{U\psi_i}$$

is another probability measure on the real line, with the same mean and standard deviation as the one above. Thus, by Chebyshev's inequality, the integral of this probability measure over the complement of J is less than or equal to $((M/n)/d)^2$, where d is the distance of I from the complement of J. In other words,

$$\frac{1}{\|\psi_i\|_1} \int\limits_{\mathbb{R}-J} \widetilde{U\psi_i} \le \left(\frac{Md}{n}\right)^2$$

or writing $(Md)^2 = c$,

$$\int_{\mathbb{R}} (1 - \chi_J) \widetilde{U\psi_i} \le \frac{c}{n^2} \, \|\psi_i\|_1$$

or equivalently

$$\int_{X} (1 - \chi_J(O)(x)) (U\psi_i)(x) \, dx \le \frac{c}{n^2} \, \|\psi_i\|_1.$$

Since the integrand is nonnegative, this implies

$$\|(1 - \chi_J(O))U\psi_i\|_1 \le \frac{c}{n^2}\|\psi_i\|_1$$

which is (1), as desired.

Combining these three lemmas, the converse follows.

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