Equivalence classes for large deviations

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We show the existence of equivalence classes for large deviations. Stochastic dynamics within an equivalence class share the same large deviation properties.

KEY TAKEAWAYS

- An equivalence relation for stochastic dynamics is defined. Stochastic dynamics that belong to the same equivalence class have the same large deviations.
- Stochastic dynamics can be factored into an equilibrium and a nonequilibrium part. The equilibrium part is common to all elements of an equivalence class.
- Large deviations can be expressed in terms of a scalar field defined on the equivalence classes. The symmetry of this field gives rise to the symmetries of the fluctuations theorems.
- The large deviations of an equilibrium dynamics determine the large deviations of all the nonequilibrium dynamics within its equivalence class.

I. FRAMEWORK

A. Markov chains

We consider a Markov chain characterized by a transition matrix \( P = (P_{ij}) \in \mathbb{R}^{N \times N} \) on a finite state space. The operator \( P \) is stochastic, i.e., it is non-negative (\( P \geq 0 \)) and its rows sum to one (\( \sum_j P_{ij} = 1 \)). We assume that the Markov chain is primitive, i.e., there exists an \( n_0 \) such that \( P^{n_0} \) has all positive entries. This guarantees that \( P \) has a unique stationary distribution \( \pi \) such that \( \pi P = \pi \).

For further reference, we note that a non-negative matrix can be transformed into a stochastic matrix. Indeed, consider a non-negative matrix \( A \) and denote its Perron root by \( \chi \) and its right Perron vector by \( x \). Then if \( D = \text{diag}(x_1, \ldots, x_N) \) we have that

\[
P = \frac{1}{\chi} D^{-1} AD
\]

is a stochastic matrix.

B. Thermodynamic description

A Markov chain \( P \) defines an equilibrium dynamics when

\[
P_{i_1 i_2} \cdots P_{i_n i_1} = P_{i_1 i_n} \cdots P_{i_2 i_1} \quad \text{for any finite sequence} \quad (i_1, i_2, \ldots, i_n).
\]

In this case, no probability flux is present at the stationary state.

When the conditions (2) are not satisfied we are in presence of a nonequilibrium dynamics. In this case, probability fluxes circulate through the system and generate thermodynamic forces or affinities. The affinities can be measured by the breaking of detailed balance along cyclic paths \( c = (i_1, i_2, \ldots, i_n) \) as

\[
\frac{P_{i_1 i_2} \cdots P_{i_n i_1}}{P_{i_1 i_n} \cdots P_{i_2 i_1}} = \exp (A_c).
\]

However, Schnakenberg demonstrated that only a subset of these affinities are independent. He also showed how to identify a basis of affinities \( \mathbf{A} = (A_1, \ldots, A_i, \ldots, A_M) \) based on the concept of fundamental chords. A summary of his theory is presented in the Appendix.
II. THERMODYNAMIC DECOMPOSITION OF STOCHASTIC DYNAMICS

Stochastic dynamics can be brought into a "thermodynamic form" through a similarity transform. This form decomposes the dynamics into an equilibrium and a nonequilibrium part. It is thus expressed in terms of two operators \( E \) and \( Z \), defined as

\[
E_{ij}[P] = \sqrt{P_{ij}P_{ji}}
\]

and

\[
Z_{ij}(\mu) = \begin{cases} 
\exp(\pm \mu_i/2) & \text{if the transition } i \to j \text{ is a fundamental chord } l \text{ in the positive (negative) orientation,} \\
1 & \text{otherwise.} 
\end{cases}
\]

The operator \( E \) is symmetric, \( E = E^T \), while \( Z(\mu) = Z^T(-\mu) \).

We have the following

**Proposition.** A stochastic matrix \( P \) with affinities \( A \) is similar to

\[
E[P] \circ Z(A),
\]

where \( X \circ Y \) denotes the Hadamard product: \((X \circ Y)_{ij} = X_{ij}Y_{ij}\).

**DEMONSTRATION:** We consider the similarity transform

\[
P' = UPU^{-1}
\]

with \( U = \text{diag}(u_1, \ldots, u_N) \). Therefore \( P'_{ij} = P_{ij}(u_i/u_j) \). We choose the elements \( u_i \) such that

\[
\frac{u_i}{u_j} = \left( \frac{P_{ji}}{P_{ij}} \right)^{1/2}
\]

for all the transitions \( i \equiv j \) that do not correspond to a chord. We have thus constrained the ratios \( \frac{u_i}{u_j} \) along the edges of the maximal tree. By construction, this provides a consistent set of equations whose solution is determined up to a multiplicative factor.

The elements of \( P' \) then take the values

\[
P'_{ij} = \sqrt{P_{ij}P_{ji}} = E_{ij}[P]Z_{ij}
\]

if the transition \( i \to j \) is not a chord.

The elements corresponding to chords are obtained as follows. Consider the chord \( l \equiv i_1 \to i_1 \) (in the positive orientation) and its fundamental cycle \( c_l = (i_1, \ldots, i_1) \). We have the identity

\[
\prod_{k=1}^l \frac{u_{i_{k+1}}}{u_{i_k}} = \prod_{k=1}^{l-1} \frac{u_{i_{k+1}}}{u_{i_k}} = 1,
\]

where \( i_{l+1} \equiv i_1 \). By construction, a fundamental cycle \( c_l \) only contains its associated chord \( l \). Hence, using formulas (3) and (7), we have

\[
\frac{u_{i_1}}{u_{i_1}} = \left( \frac{P_{i_1i_1}}{P_{i_1i_1}} \right)^{1/2} \prod_{k=1}^l \left( \frac{P_{i_{k+1}i_1}}{P_{i_ki_1}} \right)^{1/2} = \left( \frac{P_{i_1i_1}}{P_{i_1i_1}} \right)^{1/2} e^{A_l/2}.
\]

Accordingly, the operator element associated with the chord \( l \) reads

\[
P'_{i_1i_1} = \sqrt{P_{i_1i_1}P_{i_1i_1}} e^{A_l/2} = E_{i_1i_1}[P]Z_{i_1i_1}(A).
\]

Similarly, \( P'_{i_1i_1} = \sqrt{P_{i_1i_1}P_{i_1i_1}} \exp(-A_l/2) = E_{i_1i_1}[P]Z_{i_1i_1}(A) \) for the negative orientation. \( \square \)

We call (6) the thermodynamic form of \( P \). The operator \( E \) captures the equilibrium part of the dynamics while \( Z \) measures the nonequilibrium conditions. This form is symmetric for equilibrium dynamics, while the symmetry is explicitly broken by the affinities out of equilibrium.

Note that this form preserves the eigenvalues of \( P \) as well as its affinities. Also, the same similarity transform \( U \) brings a non-negative matrix into its thermodynamic form.
III. EQUIVALENCE RELATION

The thermodynamic decomposition (6) structures the space of stochastic dynamics into equivalence classes. We define the equivalence relation

\[ P \sim H \quad \text{if there exists a factor } \gamma \text{ such that } E[P] = \gamma E[H]. \] (8)

This relation is reflexive, symmetric, and transitive. It thus forms a partition of the space of stochastic dynamics: every dynamics belongs to one and only one equivalence class.

We can parametrize the elements of an equivalence class. For simplicity, we work in the thermodynamic representation (6) and use the equivalence (1) between non-negative and stochastic matrices. We then have the

**Proposition.** The equivalence class \([P]\) is composed of all the dynamics

\[ E[P] \circ Z(\mu), \] (9)

where the parameters \(\mu\) can take any values in \(\mathbb{R}^M\).

**Demonstration:** All elements in \([P]\) can be written in the form (9). This results from Proposition 1 and the definition of \(Z\). Conversely, elements of the form (9) belong to \([P]\). □

Note that an equivalence class covers all possible thermodynamic conditions. Among these, the dynamics \(E\) is the unique equilibrium dynamics; it also defines the common structure for all elements in the class.

In the following we show that the equivalence relation (8) plays a pivotal role in understanding large deviations.

IV. LARGE DEVIATIONS AND THERMODYNAMIC FORM

We define a scalar field \(\rho\) over the equivalence class \([P]\) as

\[ \rho(P, \mu) = \text{spectral radius of } E[P] \circ Z(\mu). \] (10)

It has the symmetry property

\[ \rho(P, \mu) = \rho(P, -\mu). \] (11)

Large deviations can be expressed in terms of the field \(\rho\). Indeed, the large deviations of \(P\) are obtained as (minus the logarithm of) the largest eigenvalue of

\[ P \circ Q(\lambda), \] (12)

where \(Q(\lambda)\) is a non-negative operator that measures the physical quantities of interest. Using that \(E[Q] = I\), where \(I\) is the identity matrix, and that \(Z(x) \circ Z(y) = Z(x + y)\), the thermodynamic form of (12) reads

\[ E[P] \circ Z[A + q(\lambda)]. \] (13)

The function \(q\) is readily calculated by looking at the transition probabilities of \(Q\) along cycles. The large deviations are then given by \(\rho[P, A + q(\lambda)]\).

**Example:** Large deviations of the entropy production. In this case the operator \(Q(\lambda)\) takes the form

\[ Q_{ij}(\lambda) = \left( \frac{P_{ij}}{P_{ij}} \right)^\lambda. \]

In the thermodynamic representation \(P \circ Q(\lambda)\) reads

\[ E[P] \circ Z[(1 - 2\lambda)A]. \]

Therefore, the large deviations of the entropy production probe the dynamics in \([P]\) with affinities \((1 - 2\lambda)A\). They are thus given by \(\rho[P, (1 - 2\lambda)A]\). Note that the fluctuation symmetry \(\lambda \rightarrow 1 - \lambda\) follows from the symmetry (11).
V. LARGE DEVIATIONS WITHIN AN EQUIVALENCE CLASS

For concreteness, we consider the large deviations of the thermodynamic currents. They are measured by the operator \( Q(\lambda) = Z(-2\lambda) \). Therefore, they are obtained from \( \rho(P, A - 2\lambda) \). Note that the fluctuation symmetry \( \lambda \rightarrow A - \lambda \) follows from the symmetry (11).

We have the

**Theorem.** Dynamics within an equivalence class share the same large deviations.

**Demonstration:** Note that \( \rho(P, \mu) = \rho(P', \mu) \) if \( P \) and \( P' \) are in the same equivalence class. Therefore, the large deviations of \( P, \rho(P, A - 2\lambda) \), are obtained from the large deviations of \( P', \rho(P', A' - 2\lambda') \), by the parameter transformation \( \lambda' \rightarrow \lambda + (A' - A)/2 \). □

**Corollary.** The large deviations of the equilibrium dynamics \( E[P] \) determine the large deviations of the whole equivalence class \( [P] \).

The equilibrium dynamics \( E[P] \) thus presents the same large deviation properties as \( P \). In this sense, \( E[P] \) is the natural equilibrium state of \( P \) from a dynamical viewpoint.3

**Disclaimer.** This paper is not intended for journal publication.

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**Appendix A: Schnakenberg theory**

Schnakenberg’s theory decomposes the thermodynamical properties of stochastic dynamics into independent contributions. A graph \( G \) is associated with a stochastic dynamics as follows: each state \( i \) of the system corresponds to a vertex while the edges represent the different transitions \( i \leftrightarrow j \) allowed between the states. An orientation is given to each edge of the graph \( G \).

A graph \( G \) usually contains cyclic paths. However, not all such paths are independent. They can be expressed by a linear combination of a smaller subset of cycles, called the fundamental set, which plays the role of a basis in the space of cycles. To identify all the independent cycles of a graph we introduce a maximal tree \( T(G) \), which is a subgraph of \( G \) that satisfies the following properties:

- \( T \) contains all the vertices of \( G \);
- \( T \) is connected;
- \( T \) contains no circuit, i.e., no cyclic sequence of edges.

In general a given graph \( G \) has several maximal trees.

The edges \( l \) of \( G \) that do not belong to \( T \) are called the chords of \( T \). For a graph with \( N \) vertex and \( E \) edges, there exists \( M = E - N + 1 \) chords. If we add to \( T \) one of its chords \( l \), the resulting subgraph \( T + l \) contains exactly one circuit, \( c_l \), which is obtained from \( T + l \) by removing all the edges that are not part of the circuit. Each chord \( l \) thus defines a unique cycle \( c_l \) called a fundamental cycle.

We can formulate many important thermodynamic concepts in terms of cycles. For instance, the affinity of an arbitrary cycle \( c \) is a linear combination of the affinities of a fundamental set:

\[
A(c) = \sum_l \epsilon_l(c)A(c_l),
\]

where \( \epsilon_l(c) \) is the coefficient of \( c \) in the cycle decomposition of \( c_l \).
where the sum extends over all the chords, and $\epsilon_l(c) = \pm 1$ if $c$ contains the chord $l$ in the positive (+) or negative orientation (−), and 0 otherwise. This illustrates that the fundamental cycles constitute a basis identifying the independent contributions to the stochastic process.

1. J. Schnakenberg, Rev. Mod. Phys, 48, 571 (1976).
2. A non-negative matrix $A$ and its associated stochastic operator (1) have the same thermodynamic form, up to a multiplicative factor.
3. It does not, however, necessarily coincide with the intuitive equilibrium of the system. For example, consider a three-states dynamics $P_a$, with $P_{12} = P_{13} = P_{21} = P_{23} = 1/2, P_{31} = a, P_{32} = 1 - a$. Its thermodynamic equilibrium, from a parametric viewpoint, occurs when $a = 1/2$. However, $E[P_a]$ is not similar to $P_{1/2}$ when $a \neq 1/2$.
4. Accordingly, the maximal tree $T$ can be chosen arbitrarily because each cycle $c_l$ can be redefined by linear combinations of the fundamental cycles.