Unified framework for the second law of thermodynamics and information thermodynamics based on information geometry

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Information geometry, that is a differential geometric method of information theory, gives a natural definition of informational quantity from the projection theorem. In this letter, we report that the second law of thermodynamics can be obtained from this projection. This result implies that a calculation of the entropy production can be regarded as an optimization problem. Moreover, recent results in information thermodynamics can be obtained in a unified way. This geometric picture of the second law provides the hierarchy of thermodynamic inequalities and additivity of the second laws.

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Information geometry\textsuperscript{1,2} is a theory of differential geometry for organizing various results in information theory, probability theory and statistics. The application of information geometry has been discussed in a variety of fields including the machine learning\textsuperscript{3}, neuroscience\textsuperscript{4}, statistical physics\textsuperscript{5,6} and thermodynamics\textsuperscript{7,10}. In an application of information geometry, the projection theorem\textsuperscript{11,12} has a crucial role. For example, the projection theorem provides the conventional definitions of information quantities such as the mutual information, the transfer entropy and the integrated information\textsuperscript{2,13,14}.

In last two decades, the second law of thermodynamics has been discussed in the field of stochastic thermodynamics\textsuperscript{15,16}. In stochastic thermodynamics, the fluctuation theorem\textsuperscript{17,18} leads to an expression of the second law by the Kullback-Leibler divergence\textsuperscript{19}. Recent results in information thermodynamics\textsuperscript{20}, such as the second law of information thermodynamics\textsuperscript{21,31}, are also based on the Kullback-Leibler divergence\textsuperscript{32}. Although the Kullback-Leibler divergence is strongly related to information geometry, an information geometric interpretation of the second law has been elusive\textsuperscript{33,41}.

In this letter, we show that the second law of thermodynamics can be derived from the projection theorem. To introduce a manifold related to reversible dynamics, the entropy production can be considered as the minimum length from this manifold. This fact leads to a novel interpretation that a calculation of the entropy production can be regarded as an optimization problem to minimize the length.

In addition, we show that the second law of information thermodynamics can also be derived from the projection onto the manifold related to local reversibility of bivariate dynamics. From the inclusion property of manifolds, we obtain a hierarchy that the bound by information thermodynamics is always tighter than the bound by thermodynamics. Moreover, the additivity of the second laws gives a nontrivial quadrangle in non-Euclidean space of information geometry. We illustrate these results by the two spins model.

The projection theorem.– We first introduce the projection theorem in information geometry\textsuperscript{11,12}. We consider a geometry of the joint probability $p_{S}(s)$, where $S = \{s_1, ..., s_N\}$ is the set of random variables and $s = \{s_1, ..., s_N\}$ is the set of events. The set of probabilities gives a manifold, and the probability $p_{S}(s)$ corresponds to a point on this manifold. If we discuss the projection theorem in information geometry, the metric is given by the Fisher information, and the connection is given by the dual affine connections\textsuperscript{11}.

We here consider a submanifold $\mathcal{M}$ that is the subset of probabilities, and an optimization problem to minimize the Kullback-Leibler divergence between $p_{S}(s)$ and a probability $q_{S}(s)$ on the manifold $\mathcal{M}$

$$\min_{q_{S}\in \mathcal{M}} D(p||q),$$

where $D(p||q) = \sum_{s} p_{S}(s) \ln [p_{S}(s)/q_{S}(s)]$ is the Kullback-Leibler divergence between two probabilities $p_{S}$ and $q_{S}$. If the manifold $\mathcal{M}$ is flat, this optimization prob-
The condition of the flatness is given by the linear constraints of \( \theta \)-coordinate, which is parameters of the exponential family \([1]\). For any probabilities \( q_S \) on the flat manifold \( M \), we have the generalized Pythagorean theorem
\[
D(p_S || q_S) = D(p_S || q^*_S) + D(q^*_S || q_S). 
\]
(3)

It indicates that the dual geodesic connecting \( p \) and \( q^* \) is orthogonal to the geodesic connecting \( q^* \) and \( q \), and the Kullback-Leibler divergence \( D(p_S || q_S) \) gives the minimum length from the manifold \( M \) \([2]\) (see also Fig. 1).

This projection theorem is useful to define informational quantities. We here show two examples to define the mutual information \( I(X; Y) \) and the measure of information flow known as the transfer entropy \( TE(Y \rightarrow X) \) \([13]\), which appear in the second law of information thermodynamics \([21, 24]\). At first, we consider the manifold related to statistical independence \( M_I : q_S(s) = q_X(x)q_Y(y) \) with \( S = \{X, Y\} \), \( q_X(x) = \sum_y q_S(s) \) and \( q_Y(y) = \sum_x q_S(s) \). We obtain the mutual information from the projection onto this manifold \( M_I \) \([2]\),
\[
\min_{q_S \in M_I} D(p_S || q_S) = I(X; Y),
\]
(4)
\[
I(X; Y) = H(X) + H(Y) - H(S),
\]
(5)
where \( H(S) \) is the Shannon entropy defined as \( H(S) = -\sum_s p_S(s) \log p_S(s) \).

Next, we consider the transition from \( X \) to \( X' \) under the condition of \( Y \), the transition probability is given by \( p_{X' | X} \cdot y(x', y) = p_S(s)/\sum s p_S(s) \) with \( S = \{X', X, Y\} \). The transfer entropy \( TE(Y \rightarrow X) \) can be obtained from the projection onto manifold related the conditional independence in the transition probability \( M_T : q_X(x, y | x', y) = q_X(x') q_Y(y | x') \) \([13]\),
\[
\min_{q_S \in M_T} D(p_S || q_S) = TE(Y \rightarrow X),
\]
(6)
\[
TE(Y \rightarrow X) = I(\{X, X'; Y\} | X) - I(X; Y)
= I(X'; Y | X). 
\]
(7)

The second law of thermodynamics.- We here show that the entropy production can be obtained from the projection theorem. We consider the manifold of the path probability \( p_{Z,Z'}(z, z') \), where \( Z \) and \( Z' \) are random variables of the state of the system \( Z \) at time \( t \) and \( t + dt \), respectively. The transition probability is given by the conditional probability \( T(z'|z) = p_{Z,t \rightarrow t+1}(z'|z) \). The condition of reversibility is given by the detailed balance \( T(z'|z)p_Z(z) = T(z|z')p_{Z,t \rightarrow t+1}(z') \), or equivalently \( p_{Z,t \rightarrow t+1}(z|z') = T(z|z') \).

We introduce the reversible manifold that backward dynamics from \( Z' \) to \( Z \) are driven by the transition probability \( T \),
\[
M_R : q_{Z|Z'}(z|z') = T(z|z').
\]
(8)

This manifold \( M_R(p_{Z,Z'}) \) is a function of \( T = p_{Z,Z'} \).

If the joint probability is on this manifold \( p_{Z,Z'} \in M_R(p_{Z,Z'}) \), dynamics of \( Z \) are reversible in time \( T(z'|z)p_Z(z) = T(z|z')p_{Z,t \rightarrow t+1}(z') \).

We consider the projection onto the manifold \( M_R \).

In the case \( q_{Z,Z'}(z, z') = T(z|z')p_{Z,t \rightarrow t+1}(z') \), the following Pythagorean theorem holds for any \( q_{Z,Z'} \in M_R \),
\[
D(p_{Z,Z'} || q_{Z,Z'}) = D(p_{Z,Z'} || q^*_{Z,Z'}) + D(q^*_{Z,Z'} || q_{Z,Z'}).
\]
(9)

The second term \( D(q^*_{Z,Z'} || q_{Z,Z'}) = D(p_{Z,Z'} || q_{Z,Z'}) \) can be interpreted as the degree of freedom in the probability distribution of \( Z' \). From this Pythagorean theorem, we have a unique solution \( q^*_{Z,Z'} \), i.e.,
\[
\min_{p_{Z,Z'} \in M_R} D(p_{Z,Z'} || q_{Z,Z'}) = D(p_{Z,Z'} || q^*_{Z,Z'}).
\]

From stochastic thermodynamics, the Kullback-Leibler divergence \( D(p_{Z,Z'} || q_{Z,Z'}) \) is equal to the entropy production \( \sigma^Z_{\text{tot}} \) \([19]\),
\[
D(p_{Z,Z'} || q_{Z,Z'}) = \sigma^Z_{\text{tot}} = \sigma^Z_{\text{sys}} + \sigma^Z_{\text{bath}},
\]
(10)
\[
\sigma^Z_{\text{sys}} = H(Z') - H(Z),
\]
(11)
\[
\sigma^Z_{\text{bath}} = \sum_{z,z'} p_{Z,Z'}(z, z') \ln \frac{T(z'|z)}{T(z|z')},
\]
(12)
where \( \sigma^Z_{\text{sys}} \) is the entropy change of the system \( Z \), and \( \sigma^Z_{\text{bath}} \) is the entropy change of the heat bath attached to the system \( Z \). From the projection theorem, a calculation of the entropy production can be regarded as an optimization problem (see also Fig. 2),
\[
\sigma^Z_{\text{tot}} = \min_{q_{Z,Z'} \in M_R} D(p_{Z,Z'} || q_{Z,Z'}).
\]
(13)

The entropy production is nonnegative, because the Kullback-Leibler divergence is nonnegative \( D(p || q) \geq 0 \). This nonnegativity is the second law of thermodynamics. If and only if the path probability is on the reversible manifold, the entropy production vanishes.

The result \( (13) \) gives a novel interpretation of the second law of thermodynamics from a view point of the learning process. In information geometry, the learning process is formalized as the reduction process of the minimum length between the distribution \( p_t \) in each iteration \( t \) and the manifold of the statistical model \( M_t \), i.e., \( \lim_{t \rightarrow 0} \min_{p_t \in M_t} D(p_t || q) \rightarrow 0 \). In the same way, we can interpret the equilibrium process \( \lim_{t \rightarrow 0} \sigma^Z_{\text{tot}} \rightarrow 0 \) as the learning process of reversibility \( \lim_{t \rightarrow 0} \min_{q_{Z,Z'} \in M_R} D(p_{Z,Z'} || q_{Z,Z'}) \rightarrow 0 \).

Our formalization would be useful to detect the entropy production from the experimental data. Based on our framework, we can use optimization tool to calculate the entropy production in parallel with an estimation of informational quantities such as the mutual information and the transfer entropy \([14]\).

The second law of information thermodynamics.- Recent studies of stochastic thermodynamics reveal a deep
connection between thermodynamics and information theory. If we consider the subsystem interacting other systems, informational quantities such as mutual information and the transfer entropy between them appears in a generalization of the second law [21, 24]. This generalization is called as the second law of information thermodynamics. We show that the second law of information thermodynamics can also be derived from the projection theorem in a unified way [47].

We here consider the situation that $\mathcal{Z}$ is given by random variables of two systems $\mathcal{X}$ and $\mathcal{Y}$, i.e., $\mathcal{Z} = \{X, Y\}$ and $\mathcal{Z}' = \{X', Y'\}$. We assume the bipartite condition $c_{\text{BI}}$ that the transition probability $T(z'|z) = T(x', y'|x, y)$ is given by two transition probabilities $T(z'|z) = T_X^X(x'|x)T_Y^Y(y'|y)$. The condition of local reversibility in the system $\mathcal{X}$ is given by $p_{X|Z}(x|z') = T_Y^Y(x|z')$.

The second law of information thermodynamics for the subsystem $\mathcal{X}$ is given by the inequality of the partial entropy changes and information flow $\Theta^{X\to Y}$ from $\mathcal{X}$ to $\mathcal{Y}$,

$$\sigma^{\mathcal{X}}_{\text{sys}} + \sigma^{\mathcal{X}}_{\text{bath}} \geq \Theta^{X\to Y},$$  
$$\sigma^{\mathcal{X}}_{\text{sys}} = H(X') - H(X),$$  
$$\sigma^{\mathcal{X}}_{\text{bath}} = \sum_{z, z'} p_{Z, Z'}(z, z') \ln \frac{T_y^Y(x'|x)}{T_y^Y(x|x')},$$  
$$\Theta^{X\to Y} = I(X'; Y, Y') - I(X; Y, Y').$$  

The term of information flow includes the (backward) directed information $I(X'; \{Y, Y'\}) = I(X; \{Y, Y'\})$, which is given by the sum of mutual information at time $t$ ($t + dt$) and the (backward) transfer entropy, i.e., $I(X; \{Y, Y'\}) = I(X; Y) + \text{TE}(X \to Y)$, $I(X'; \{Y, Y'\}) = I(X'; Y') + \text{BTE}(X \to Y)$ with $\text{BTE}(X \to Y) \equiv I(X'; Y|Y')$. If dynamics are given by the master equation with the bipartite condition $c_{\text{BT}}$, information flow is equivalent to the learning rate

$$\Theta^{X\to Y} = I(X'; Y) - I(X; Y') = I(X'; Y') - I(X; Y').$$  

up to order $O(dt^2)$ [23, 24].

We here introduce the local reversible manifold of $\mathcal{X}$ that backward dynamics from $\mathcal{Z}'$ to $\mathcal{X}$ are driven by the transition probability $T^X$,

$$\mathcal{M}_{\mathcal{LR}}^X : q_{X|Z}(x|z') = T_{y'}^X(x|z').$$  

The reversible manifold is the submanifold of the local reversible manifold $\mathcal{M} \subset \mathcal{M}_R$. If the joint probability $p_{Z, Z'}$ is on this manifold, dynamics of $\mathcal{X}$ are locally reversible in time. In the case $q_{X|Z}(x|z') = T_{y'}^X(x|z')p_{Y, Z'}(y, z')$, the following Pythagorean theorem holds for any $q_{Z, Z'} \in \mathcal{M}_{\mathcal{LR}}^X$,

$$D(p_{Z, Z'}||q_{Z, Z'}) = D(p_{Z, Z'}||q_{X, Z'}) + D(q_{X, Z'}||q_{Z, Z'}).$$  

The second term $D(p_{Z, Z'}||q_{Z, Z'}) = D(p_{Y, Z'}||q_{Y, Z'})$ can be interpreted as the degree of freedom in the probability distribution of $Y$ and $Z'$.

The second law of information thermodynamics can be obtained from the projection onto the local reversible manifold, because the Kullback-Leibler divergence $D(p_{Z, Z'}||q_{Z, Z'})$ is equal to the partial entropy production,

$$D(p_{Z, Z'}||q_{Z, Z'}) = \sigma^{\mathcal{X}}_{\text{partial}} = \sigma^{\mathcal{X}}_{\text{sys}} + \sigma^{\mathcal{X}}_{\text{bath}} - \Theta^{X\to Y}.$$  

Then, the second law of information thermodynamics can also be related to the optimization problem

$$\sigma^{\mathcal{X}}_{\text{partial}} = \min_{q_{Z, Z'} \in \mathcal{M}_{\mathcal{LR}}^X} D(p_{Z, Z'}||q_{Z, Z'}).$$  

If and only if the path probability is on the local reversible manifold, the partial entropy production vanishes.

Hierarchy of the second laws. We here show that our geometric interpretation of the second laws provides the hierarchy of the second laws. From the inclusion property of manifolds $\mathcal{M} \subset \mathcal{M}_R$, we obtain

$$\min_{p_{Z, Z'} \in \mathcal{M}} D(p_{Z, Z'}||q_{Z, Z'}) \geq \min_{p_{Z, Z'} \in \mathcal{M}_{\mathcal{LR}}^X} D(p_{Z, Z'}||q_{Z, Z'}),$$

or equivalently

$$\sigma^{X}_{\text{total}} \geq \sigma^{X}_{\text{partial}}.$$  

This result gives the hierarchy of the second laws such that the second law of information thermodynamics always gives a tighter bound than the second law of thermodynamics (see also Fig.3).

Moreover, if the total system is consist of multiple systems $\mathcal{Z}_1, \mathcal{Z}_2, \ldots, \mathcal{Z}_N$, we obtain the hierarchy for the two subsets $\{Z_{n_1}, \ldots, Z_{n_k}\} \subset \{Z_{m_1}, \ldots, Z_{m_k}\}$ as

$$\sigma^{Z_{m_1}, \ldots, Z_{m_k}} \geq \sigma^{Z_{n_1}, \ldots, Z_{n_k}}.$$  

$$\sigma^{X}_{\text{partial}} \geq \sigma^{X}_{\text{partial}}.$$  

$$\sigma^{X}_{\text{partial}} \geq \sigma^{X}_{\text{partial}}.$$
because of the inclusion property \( M_{LR}^{Z_{m_1},\ldots,Z_{m_i}} \subset M_{LR}^{Z_{n_1},\ldots,Z_{n_k}} \). This hierarchy of the second laws is useful to apply information thermodynamics to complex system. We have a lot of the second laws for complex system, because the second law of information thermodynamics is derived for any partition of the system. This hierarchy indicates that we only need to investigate the inclusion property of manifolds corresponding to the second laws to grasp the relationship between them.

The hierarchy of the second laws (22) is related to the second law of information thermodynamics for the subsystem \( \mathcal{Y} \). Under the bipartite condition for time-reversal trajectories \( C_{BI}^* : p_{Z;Z'}(z|z') = p_{X;X'}(x|x')p_{Y;Y'}(y|z') \), we exactly obtain the additivity of the entropy production,

\[
\sigma_{tot}^{\mathcal{Z}} = \sigma_{partial}^{\mathcal{X}} + \sigma_{partial}^{\mathcal{Y}},
\]

because the difference \( \sigma_{partial}^{\mathcal{X}} + \sigma_{partial}^{\mathcal{Y}} - \sigma_{tot}^{\mathcal{Z}} \) is given by the Kullback-Leibler divergence\( D(p_{Z;Z'}||p_{X;X'}p_{Y;Y'}) \). Thus, Eq. (22) is equivalent to the second law of information thermodynamics for the subsystem \( \mathcal{Y} \),

\[
\sigma_{partial}^{\mathcal{Y}} \geq 0.
\]

From the point of view of information geometry, the additivity (24) gives a nontrivial quadrangle (see also Fig. 4). The additivity gives the relationship of the Kullback-Leibler divergence

\[
D(p,Z;Z') = D(p,Z;\|q_{Z;Z'}) + D(p,Z;\|q_{Z;Z'}).
\]

\( D(p,q;\|q^*) = D(q^*;\|q) + D(p;\|q^*) \)

\( D(p,q;\|q^*) = D(q^*;\|q) \)

From the Pythagorean theorem (22), we have the following relationship

\[
D(p,Z;\|q^*_{Z;Z'}) = D(q^*_{Z;Z'};\|q_{Z;Z'})
\]

and vice versa

\[
D(p,Z;\|q^*_{Z;Z'}) = D(q^*_{Z;Z'};\|q_{Z;Z'})
\]

which means that the parallel sides of a quadrangle have the same length. We call these conditions (27) and (28) as the rectangle in information geometry. This rectangle is not so trivial because information geometry is non-Euclidean geometry. The projections onto three manifolds itself are not the necessary and sufficient condition of the rectangle.

Under the conditions of the additivity \( C_{BI} \cap C_{BI}^* \), we obtain the relationship between manifolds

\[
M_{R} = M_{LR}^{X} \cap M_{LR}^{Y}.
\]

This condition might be important for the rectangle in information geometry.

Example.— We illustrate our results by the two spins model. Let \( Z = \{S_1, S_2\} \) and \( Z' = \{S_3, S_4\} \) be random variables of two spins at time \( t \) and \( t + dt \), respectively. The spin has the binary state \( s_i \in \{0,1\} \). The path probability of the spin state is generally given by the exponential family even in nonequilibrium dynamics,

\[
p^\theta_{Z;Z'}(s) = \exp \left[ \sum_i s_i \hat{\theta}_i + \sum_{i<j} s_is_j \hat{\theta}_{ij} + \sum_{i<j<k} s_is_js_k \hat{\theta}_{ijk} + \sum_{i<j<k<l} s_is_js_k \hat{\theta}_{ijkl} - \phi_{Z;Z'}(\hat{\theta}) \right].
\]
where $\hat{\theta}$ is the set of parameters, and $\phi_{Z,Z'}(\hat{\theta})$ is the normalization factor that satisfies $\sum_s \phi_{Z,Z'}(s) = 1$. The parameter $\hat{\theta}$ in $p_{Z,Z'}^\theta(s)$ gives a coordinate called as $\theta$-coordinate. The number of the elements in $\theta$ is $(2^4 - 1) = 15$, then the probability $p_{Z,Z'}^\theta(s)$ can be represented by $\theta$-coordinate in 15-dimensional manifold.

The both bipartite conditions $C_{BI}$ and $C_{BI}'$ gives a constraint in 15-dimensional manifold. The bipartite conditions are given by

$$C_{BI} : \theta^{34} = \theta^{134} = \theta^{234} = \theta^{1234} = 0, \quad (31)$$

$$C_{BI}' : \theta^{12} = \theta^{123} = \theta^{1234} = 0, \quad (32)$$

which are 7-dimensional constraints in the manifold $[48]$. Under the both bipartite conditions, three-body and four-body correlations vanish.

For stochastic thermodynamics $[16]$, the ratio of the transition probability is given by the Hamiltonian difference

$$T(z'|z) = T(z|z') \exp \left[ \beta (H(z) - H(z')) \right], \quad (33)$$

where $H(z)$ is the Hamiltonian of two spin states $z = (s_1, s_2)$, and $\beta$ is the inverse temperature. The entropy change in the bath $\sigma^B_{\text{bath}}$ is calculated as $\sigma^B = -\beta Q$, where $Q := \sum_s p^2_{Z,Z'}(s) (H(z') - H(z))$ is the expected value of the heat dissipation. If the distribution of probability at time $t$ is given by the canonical distribution $p_Z(z) \propto \exp[-\beta H(z)]$, the canonical distribution gives the stationary distribution $p_Z = p_{Z'}$ and the detailed balance $T(z'|z) p_Z(z) = T(z|z') p_{Z'}(z')$ holds.

To calculate the entropy production, we consider the reversible manifold $\mathcal{M}_R$. A coordinate $\theta$ represents a probability on the reversible manifold $q_{Z,Z'}(s) = p_{Z,Z'}^\theta(s) \in \mathcal{M}_R$. Under the both bipartite conditions $C_{BI}$ and $C_{BI}'$, the condition of the reversible manifold is given by $\theta$ as a function of $\hat{\theta}$,

$$\mathcal{M}_R : \theta^1 = \hat{\theta}^3, \quad \theta^2 = \hat{\theta}^4, \quad \theta^{23} = \hat{\theta}^{14}, \quad \theta^{24} = \hat{\theta}^{24}, \quad \theta^{13} = \hat{\theta}^{13}, \quad \theta^{14} = \hat{\theta}^{23}, \quad (34)$$

The reversible manifold is flat, because the condition of the flatness is given by the linear constraints $A \theta = b$ $[2]$. The condition of the local reversible manifolds are also given by the linear constraint of $\theta$ $[48]$,

$$\mathcal{M}^X_{LR} : \theta^1 = \hat{\theta}^3, \quad \theta^{13} = \hat{\theta}^{13}, \quad \theta^{14} = \hat{\theta}^{23}, \quad (35)$$

$$\mathcal{M}^Y_{LR} : \theta^2 = \hat{\theta}^4, \quad \theta^{24} = \hat{\theta}^{24}, \quad \theta^{23} = \hat{\theta}^{14}. \quad (36)$$

The intersection of these two manifolds is the reversible manifold $\mathcal{M}_R = \mathcal{M}^X_{LR} \cap \mathcal{M}^Y_{LR}$ under the both bipartite conditions.

The entropy production and the partial entropy production are calculated as the optimization problems $[13]$ and $[44]$ for the set of parameters $\theta$. For each experimental observation of the path probability characterized by $\hat{\theta}$, we can calculate to minimize $D(p_{Z,Z'}^\theta || p_{Z,Z'}^\theta)$ on the manifold characterized by $\theta$ for an experimental estimation of the (partial) entropy production.

Conclusion and discussion.— In information geometry, this optimization problem of the Kullback-Leibler divergence is well studied as a statistical inference $[50]$, a hypothesis testing $[51]$, and an expectation-maximization algorithm $[52]$. Our framework would provide an information-geometric estimation of the entropy production by using a conventional optimization tool.

By applying information-geometric framework, we clarify the relationship between the second law of thermodynamics and information thermodynamics. This result is complement to other geometric expressions of the second law, such as the principle of Carathéodory $[54]$ and the maximum entropy thermodynamics $[55]$, while our result is based on the manifold of reversibility unlike the other.

Variants of the second laws could be derived from the selection of $T$ that gives another manifold. For example, if we consider $T$ of the dual dynamics $[16]$ we would obtain the generalized second law for non-equilibrium steady state $[53]$. The hierarchy does not apply only to the second laws of information thermodynamics. Our framework gives the hierarchy for variants of the second laws by using the inclusion property of manifolds corresponding to selections of $T$.

Because the second law of information thermodynamics would be essential for biochemical information processing $[21, 57, 62]$, this work would give a geometric insight into biochemical information processing. It is also interesting that the concept of the second law of information thermodynamics is similar to the integrated information theory $[63, 64]$ in this information-geometric framework $[13, 14]$.

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We also obtain the second law of thermodynamics under feedback control in a unified way. See Supplemental Material, for the detail.

We here consider the situation that the time evolution of the system $X$ depend on the memory $M$. Let $X$ and $X'$ be random variables of the system $X$ at time $t$ and $t+dt$, respectively. Let $M$ be a random variable of the memory $M$. The transition probability of $X$ depend on the state of memory, $T^X_m(x'|x) = p_{X'|X,M}(x'|x,m)$. The condition of feedback reversibility in the system $X$ is given by $p_{X'X,M}(x'|x,m) = T^X_m(x|x')$.

The second law of thermodynamics under feedback control is given by the inequality of the partial entropy changes and the mutual information change $\Delta I$,

\begin{align}
\sigma^X_{\text{sys}} + \sigma^X_{\text{bath}} &\geq \Delta I, \\
\sigma^X_{\text{sys}} &\geq H(X') - H(X), \\
\sigma^X_{\text{bath}} &\geq \sum_{x,x',m} p_{X,X',M}(x,x',m) \ln \frac{T^X_m(x'|x)}{T^X_m(x|x')}, \\
\Delta I &\geq I(X';M) - I(X;M).
\end{align}

We here introduce the feedback reversible manifold that backward dynamics from $X'$ to $X$ are driven by the transition probability $T^X$,

\[ M_{\text{FR}} : q_{X'|X,M}(x'|x,m) = T^X_m(x|x'). \]

The feedback reversible manifold is equivalent to the reversible manifold $M_{\text{R}} = M_{\text{FR}}$, if we consider the time evolution from $Z = \{X,M\}$ to $Z' = \{X',M\}$. If the joint probability $p_{X,X',M}$ is on this manifold, dynamics of $X$...
are reversible in time under feedback control. In the case \( q_{X,X',M}^*(x, x', m) = T_m^X(x|x')p_{X',M}(x', m) \), the following Pythagorean theorem holds for any \( q_{X,X',M} \in M_{FR} \),

\[
D(p_{X,X',M}||q_{X,X',M}) = D(p_{X,X',M}||q_{X,X',M}^*) + D(q_{X,X',M}^*||q_{X,X',M}).
\] (42)

The second term \( D(q_{X,X',M}^*||q_{X,X',M}) = D(p_{X,M}||q_{X,M}) \) can be interpreted as the degree of freedom in the probability distribution of \( M \) and \( X' \).

The second law of thermodynamics under feedback control can be obtained from the projection onto the local reversible manifold, because the Kullback-Leibler divergence \( D(p_{Z,Z'}||q_{Z,Z'}^*) \) is equal to the partial entropy production,

\[
D(p_{X,X',M}||q_{X,X',M}^*) = \sigma_{\text{partial}}^X = \sigma_{\text{sys}}^X + \sigma_{\text{path}}^X - \Delta I.
\] (43)

Then, the second law of thermodynamics under feedback control can also be related to the optimization problem

\[
\sigma_{\text{partial}}^X = \min_{q_{X,X',M} \in M_{FR}} D(p_{X,X',M}||q_{X,X',M}).
\] (44)

If and only if the path probability is on the feedback reversible manifold, the partial entropy production vanishes.

II. Detailed calculations of the additivity

We here show the additivity of the entropy production Eq. (24) in the main text under the condition \( C_{BI} \). The total entropy production \( \sigma_{\text{tot}}^X \) is calculated as

\[
\sigma_{\text{tot}}^X = \sum_{z,z'} p_{Z,Z'}(z,z') \ln \frac{p_{X'|Z}(x'|z)p_{Y|Z}(y'|z)p_{Z}(z)}{p_{X'}(x')p_{Z}(z)}
\]

\[
= \sum_{z,z'} p_{Z,Z'}(z,z') \ln \frac{p_{X'|Z}(x'|z)p_{Y|Z}(y'|z)p_{Z}(z)}{p_{Y}(y)p_{Z}(z)}
\]

\[
+ \sum_{z,z'} p_{Z,Z'}(z,z') \ln \frac{p_{X,Z}(x,z)p_{Y,Z}(y,z)p_{Z}(z)}{p_{X,Z}(x,z)p_{Y,Z}(y,z)p_{Z}(z)}
\]

\[
= D(p_{Z,Z'}||q_{Z,Z'}^*) + \sum_{z,z'} p_{Z,Z'}(z,z') \ln \frac{p_{X,Z}(x,z)p_{Y,Z}(y,z)p_{Z}(z)}{p_{X,Z}(x,z)p_{Y,Z}(y,z)p_{Z}(z)}
\]

\[
= \sigma_{\text{partial}}^X + \sigma_{\text{path}}^X - D(p_{Z,Z'}||p_{X,Z}||p_{Y,Z}||p_{Z,Z'}),
\] (45)

where we used \( p_{Z,Z'} = p_{X'|Z}p_{Y'|Z}p_{Z} \) under the condition \( C_{BI} \). Under the condition \( C_{BI} \), we obtain \( p_{Z,Z'} = p_{X'|Z}p_{Y'|Z}p_{Z} \) and \( D(p_{Z,Z'}||p_{X,Z}||p_{Y,Z}||p_{Z,Z'}) = 0 \). Therefore, we can obtain the additivity of the entropy production Eq. (24) under the bipartite conditions \( C_{BI} \) and \( C_{BI} \).

III. Detailed calculations of examples in the main text

We start with the joint distribution

\[
p_{Z,Z'}^\theta(s) = \exp \left[ \sum_i s_i \theta_i + \sum_{i<j} s_{ij} \theta_{ij} + \sum_{i<j<k} s_{ijk} \theta_{ijk} + \sum_{i<j<k<l} s_{ijkl} \theta_{ijkl} - \phi_{Z,Z'}(\theta) \right],
\] (46)
where \( s = (s_1, s_2, s_3, s_4) = (x, y, x', y') \) is the spin notation with \( s_i \in \{0, 1\} \), and \( \phi_{Z, Z'}(\hat{\theta}) \) is the normalization constant. The joint distribution \( p_{Z, X'}(z, x') \) is calculated as

\[
\ln p_{Z, X'}(z, x') = \sum_{i \neq 4} s_i \hat{\theta}^i + \sum_{i < j \neq 4, j \neq 4} s_i s_j \hat{\theta}^{ij} + s_1 s_2 s_3 \hat{\theta}^{123} + \psi_{Y'}(z, x' | \hat{\theta}) - \phi_{Z, Z'}(\hat{\theta}),
\]

\[
\psi_{Y'}(z, x' | \hat{\theta}) := \ln \left[ \exp \left( \hat{\theta}^3 + \frac{s_i \hat{\theta}^{ij}}{s_j} + \frac{s_1 s_2 s_3 \hat{\theta}^{123}}{s_4} + 1 \right) \right].
\]  

(47)

Then the conditional probability \( p_{Z' | X}(x' | z) \) is calculated as

\[
\ln p_{X' | Z}(x' | z) = s_3 \hat{\theta}^3 + \frac{s_1 s_3 \hat{\theta}^{13}}{s_4} + \frac{s_2 s_3 \hat{\theta}^{23}}{s_4} + \frac{s_3 s_4 \hat{\theta}^{34}}{s_4} + \frac{s_1 s_2 s_3 \hat{\theta}^{123}}{s_4} - \phi_{X' | Z}(s_1, s_2, \hat{\theta}),
\]

\[
\phi_{X' | Z}(s_1, s_2, \hat{\theta}) := \ln \left[ \exp \left( \hat{\theta}^3 + \frac{s_1 \hat{\theta}^{13}}{s_2} + \frac{s_2 \hat{\theta}^{23}}{s_2} + \frac{s_3 \hat{\theta}^{34}}{s_2} + \frac{s_1 s_2 \hat{\theta}^{123}}{s_2} + \frac{s_1 s_4 \hat{\theta}^{134}}{s_2} + \frac{s_2 s_4 \hat{\theta}^{234}}{s_2} + \frac{s_3 s_4 \hat{\theta}^{34}}{s_2} + 1 \right) \right].
\]

(48)

The conditional probability \( p_{X' | Z, Y'}(x' | z, y') \) is calculated as

\[
\ln p_{X' | Z, Y'}(x' | z, y') = s_3 \hat{\theta}^3 + s_1 s_3 \hat{\theta}^{13} + s_2 s_3 \hat{\theta}^{23} + s_3 s_4 \hat{\theta}^{34} + s_1 s_2 s_3 \hat{\theta}^{123} + s_1 s_3 s_4 \hat{\theta}^{134} + s_1 s_2 s_4 \hat{\theta}^{234} + s_1 s_4 s_4 \hat{\theta}^{34} + \phi_{X' | Z, Y'}(s_1, s_2, s_3, s_4, \hat{\theta}),
\]

\[
\phi_{X' | Z, Y'}(s_1, s_2, s_3, s_4, \hat{\theta}) := \ln \left[ \exp \left( \hat{\theta}^3 + \frac{s_1 \hat{\theta}^{13}}{s_2} + \frac{s_2 \hat{\theta}^{23}}{s_2} + \frac{s_3 \hat{\theta}^{34}}{s_2} + \frac{s_1 s_2 \hat{\theta}^{123}}{s_2} + \frac{s_1 s_4 \hat{\theta}^{134}}{s_2} + \frac{s_2 s_4 \hat{\theta}^{234}}{s_2} + \frac{s_3 s_4 \hat{\theta}^{34}}{s_2} + 1 \right) \right].
\]

(49)

The bipartite condition \( C_{BI} \) is given by \( p_{X' | Z, Y'} = p_{X' | Z} \). From Eqs. (48) and (49), we obtain

\[
C_{BI} : \hat{\theta}^{13} = \hat{\theta}^{34} = \hat{\theta}^{234} = \hat{\theta}^{1234} = 0.
\]  

(50)

In the same way, we obtain the condition of \( C_{BI}^* \)

\[
C_{BI}^* : \hat{\theta}^{ij} = \hat{\theta}^{kl} = 0.
\]  

(51)

To clarify the relationship between \( C_{BI} \) and \( C_{BI}^* \), we can consider the permutation \((\alpha(1), \alpha(2), \alpha(3), \alpha(4)) = (3, 4, 1, 2)\). The condition of \( C_{BI}^* \) is given by the condition of \( C_{BI} \) with the permutation \( \alpha \),

\[
C_{BI}^* : \hat{\theta}^{\alpha(3)\alpha(4)} = \hat{\theta}^{\alpha(3)\alpha(4)\alpha(1)} = \hat{\theta}^{\alpha(3)\alpha(4)\alpha(2)} = 0.
\]  

(52)

Next, we discuss the reversible manifold \( M_R \). The transition probability \( T(z' | z) = p_{Z' | Z}(z' | z) \) is calculated as

\[
\ln T(z' | z) = s_3 \hat{\theta}^3 + s_4 \hat{\theta}^4 + \sum_{i < 4} s_i s_4 \hat{\theta}^{ij} + \sum_{i < 3} s_i s_3 \hat{\theta}^{ij} + s_1 s_3 s_4 \hat{\theta}^{ijkl} - \phi_{Z' | Z}(s_1, s_2, \hat{\theta}),
\]

\[
\phi_{Z' | Z}(s_1, s_2, \hat{\theta}) := \ln \left[ \exp \left( \hat{\theta}^3 + \frac{s_1 \hat{\theta}^{13}}{s_2} + \frac{s_2 \hat{\theta}^{23}}{s_2} + \frac{s_3 \hat{\theta}^{34}}{s_2} + \frac{s_1 s_2 \hat{\theta}^{123}}{s_2} + \frac{s_1 s_4 \hat{\theta}^{134}}{s_2} + \frac{s_2 s_4 \hat{\theta}^{234}}{s_2} + \frac{s_3 s_4 \hat{\theta}^{34}}{s_2} + 1 \right) \right].
\]

(53)

The conditional probability \( p_{Z | Z'}(z | z') \) is given by

\[
\ln p_{Z | Z'}(z | z') = s_1 \hat{\theta}^1 + s_2 \hat{\theta}^2 + \sum_{1 < i} s_1 s_i \hat{\theta}^{i1} + \sum_{2 < i} s_2 s_i \hat{\theta}^{2i} + \ldots
\]

\[
\phi_{Z | Z'}(s_3, s_4, \hat{\theta}),
\]
\( \phi_{Z|Z'}(s_3, s_4|\theta) \)

\[ := \ln \left[ \exp(\hat{\theta}^1 + \hat{\theta}^2 + s_3 \hat{\theta}^{23} + s_4 \hat{\theta}^{24} + \hat{\theta}^{12} + s_3 \hat{\theta}^{13} + s_4 \hat{\theta}^{14} + s_3 s_4 \hat{\theta}^{134} + s_3 \hat{\theta}^{123} + s_4 \hat{\theta}^{124} + s_3 s_4 \hat{\theta}^{1234}) \right. \\
+ \exp(\hat{\theta}^1 + s_3 \hat{\theta}^{13} + s_4 \hat{\theta}^{14} + s_3 s_4 \hat{\theta}^{134}) + \exp(\hat{\theta}^2 + s_3 \hat{\theta}^{23} + s_4 \hat{\theta}^{24} + s_3 s_4 \hat{\theta}^{234} + s_3 \hat{\theta}^{123}) + 1 \] .

The reversible manifold is defined as \( \mathcal{M}_R : q_{Z|Z'}(z|z') = p^\theta_{Z|Z'}(z|z') = T(z|z') \). The equations (53) and (54) yield

\[ \mathcal{M}_R : \theta^1 = \hat{\theta}^3, \theta^2 = \hat{\theta}^4, \theta^{23} = \hat{\theta}^{14}, \theta^{24} = \hat{\theta}^{24}, \theta^{12} = \hat{\theta}^{14}, \theta^{13} = \hat{\theta}^{13}, \theta^{14} = \hat{\theta}^{123}, \theta^{134} = \hat{\theta}^{134}, \theta^{124} = \hat{\theta}^{124}, \theta^{123} = \hat{\theta}^{123}. \] (55)

Under the both bipartite conditions \( C_{BI} \) and \( C'_{BI} \), we obtain

\[ \mathcal{M}_R : \theta^1 = \hat{\theta}^3, \theta^2 = \hat{\theta}^4, \theta^{23} = \hat{\theta}^{14}, \theta^{24} = \hat{\theta}^{24}, \theta^{13} = \hat{\theta}^{13}, \theta^{14} = \hat{\theta}^{123}, \theta^{134} = \hat{\theta}^{134}, \theta^{124} = \hat{\theta}^{124}, \theta^{123} = \hat{\theta}^{123}. \] (56)

Next, we discuss the local reversible manifold \( \mathcal{M}^Y_{LR} \). Then the transition probability \( T^Y_{Y}(x'|x) = p^\theta_{X|X'}(x'|x) \) is given by Eq. (48). The conditional probability \( p^\theta_{X|X'}(x'|x) \) is calculated as

\[ \ln p^\theta_{X|X'}(x'|x) = s_1 \hat{\theta}^1 + s_1 s_3 \hat{\theta}^{13} + s_1 s_4 \hat{\theta}^{14} + s_2 s_3 s_4 \hat{\theta}^{134} - \phi_{X|X'}(s_3, s_4|\theta), \]

\[ \phi_{X|X'}(s_3, s_4|\theta) := \ln \left[ \exp(\hat{\theta}^1 + s_3 \hat{\theta}^{13} + s_4 \hat{\theta}^{14} + s_3 s_4 \hat{\theta}^{134}) + 1 \right]. \] (57)

The local reversible manifold is defined as \( \mathcal{M}^Y_{LR} : q_{X|X'}(x|x') = p^\theta_{X|X'}(x|x') = T^Y_{Y}(x|x') \). The equations (48) and (57) yield

\[ \mathcal{M}^Y_{LR} : \theta^1 = \hat{\theta}^3, \theta^2 = \hat{\theta}^4, \theta^{23} = \hat{\theta}^{14}, \theta^{24} = \hat{\theta}^{24}, \theta^{13} = \hat{\theta}^{13}, \theta^{14} = \hat{\theta}^{123}. \] (58)

In the same way, we obtain the condition of \( \mathcal{M}^Y_{LR} \)

\[ \mathcal{M}^Y_{LR} : \theta^2 = \hat{\theta}^4, \theta^{23} = \hat{\theta}^{24}, \theta^{24} = \hat{\theta}^{14}, \theta^{134} = \hat{\theta}^{124}. \] (59)

To clarify the relationship between \( \mathcal{M}^Y_{LR} \) and \( \mathcal{M}^Y_{LR} \), we can consider the permutation \( (\alpha'(1), \alpha'(2), \alpha'(3), \alpha'(4)) = (2, 1, 4, 3) \). The condition of \( \mathcal{M}^Y_{LR} \) is given by the condition of \( \mathcal{M}^Y_{LR} \) with the permutation \( \alpha' \),

\[ \mathcal{M}^Y_{LR} : \theta^{\alpha'(1)} = \hat{\theta}^{\alpha'(3)}, \theta^{\alpha'(1)\alpha'(3)} = \hat{\theta}^{\alpha'(1)\alpha'(3)}, \theta^{\alpha'(1)\alpha'(4)} = \hat{\theta}^{\alpha'(2)\alpha'(3)}, \theta^{\alpha'(1)\alpha'(4)\alpha'(3)} = \hat{\theta}^{\alpha'(2)\alpha'(1)\alpha'(3)}. \] (60)

Under the both bipartite conditions \( C_{BI} \) and \( C'_{BI} \), we obtain

\[ \mathcal{M}^Y_{LR} : \theta^1 = \hat{\theta}^3, \theta^2 = \hat{\theta}^4, \theta^{13} = \hat{\theta}^{13}, \theta^{14} = \hat{\theta}^{24}, \theta^{123} = \hat{\theta}^{123}. \] (61)

\[ \mathcal{M}^Y_{LR} : \theta^2 = \hat{\theta}^4, \theta^{13} = \hat{\theta}^{24}, \theta^{14} = \hat{\theta}^{23}. \] (62)