Information Geometry of Dynamics on Graphs and Hypergraphs

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Abstract

We introduce a new information-geometric structure of dynamics on discrete objects such as graphs and hypergraphs. The setup consists of two dually flat structures built on the vertex and edge spaces, respectively. The former is the conventional duality between density and potential, e.g., the probability density and its logarithmic form induced by a convex thermodynamic function. The latter is the duality between flux and force induced by a convex and symmetric dissipation function, which drives the dynamics on the manifold. These two are connected topologically by the homological algebraic relation induced by the underlying discrete objects. The generalized gradient flow in this doubly dual flat structure is an extension of the gradient flows on Riemannian manifolds, which include Markov jump processes and nonlinear chemical reaction dynamics as well as the natural gradient and mirror descent. The information-geometric projections on this doubly dual flat structure lead to the information-geometric generalizations of Helmholtz-Hodge-Kodaira decomposition and Otto structure in $L^2$ Wasserstein geometry. The structure can be extended to non-gradient nonequilibrium flow, from which we also obtain the induced dually flat structure on cycle spaces. This abstract but general framework can extend the applicability of information geometry to various problems of linear and nonlinear dynamics.

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I. INTRODUCTION

Information geometry is finding and establishing its firm position as the geometric language in various scientific disciplines[1, 2]. Information geometry enables us to gain an intuitive understanding of the structures behind complicated problems of inference and estimation, for which Euclidean or Riemannian geometry is not sufficient. In addition, it can provide ways to devise new solutions and approaches for the problems[1]. While information geometry was originally developed for statistics, its applicability is now not limited to statistical problems. If notions of probability, information, or positive density appear in a problem, it is natural enough to consider its information-geometric structure.

A. Information geometry of dynamics

Dynamical systems and phenomena can be potential targets for information geometry, as we conventionally consider dynamics of probability distributions[3–5], e.g., the Fokker-Planck equations (FPE) and the Master equation, or those of positive densities, e.g., population dynamics, epidemic models, diffusion dynamics on networks, and chemical reaction dynamics[6–8]. Although applications of information geometry to those dynamics have been attempted almost since its birth, information geometry for dynamics is much less organized and principled compared with that for static problems in statistics, optimization, and others[1]. In connection with statistical inference, information geometry was employed by Amari and others to investigate Gaussian time series and autoregressive moving average (ARMA) models by representing their power spectrum as parametric manifolds[9–11]. This idea was also used to investigate linear systems[12]. Markov jump processes on finite states[1] were investigated information-geometrically by considering the hierarchical structure of joint or conditional probabilities at different time points, e.g., \( P_\theta(x_1, x_2, \cdots, x_t) \)[13]. or by introducing exponential families of Markov kernel (transition matrices), \( T_\theta(x|x') \), via exponential tilting of the kernel[14–20]. Furthermore, information geometry was applied to random walks and nonlinear diffusion equations of porous media [21, 22]. In relation to mechanics, integrable systems were associated with the dualistic gradient flow of information geometry in seminal works[23, 24], and other connections of information geometry with Lagrangian or

\[1\] Also known as Markov chains
Hamiltonian mechanics have been pursued\cite{25–27}.

\section*{B. Information measures for dynamics}

Concurrently with and almost independently of these attempts within the community of information geometry, information measures relevant to information geometry have been employed and manifested in various problems of dynamical systems and stochastic processes in information theory\cite{28}, filtering theory\cite{29, 30}, control theory\cite{31–33}, and non-equilibrium physics and chemistry\cite{34–36}. Kullback-Leibler (KL) divergence\cite{37} for probabilities and positive densities was found to work as a Lyapunov function of Markov jump processes (MJP)\cite{5}, FPE\cite{3, 38}, deterministic chemical reaction networks (CRN)\cite{39, 40}, and other dynamical systems\cite{41, 42}, the origin of which can date back to Gibbs’ H-theorem\cite{43}. Among those topics, since the establishment of chemical thermodynamics by Gibbs\cite{43} and chemical kinetics by Guldberg and Waage\cite{44}, CRN has worked as a seedbed for cultivating the theory between dynamics and divergence due to its close connection with thermodynamics\cite{45–47}. More recently, stochastic thermodynamics based on FPE and MJP has also clarified its connection to divergence and information geometry\cite{48–52}.

In addition to the KL divergence, the Fisher-information-like quantity

\[ \mathbb{I}_F[p] := \int p(r)(\nabla r \ln p(r))^2 dr \in \mathbb{R}_{\geq 0} \]  

was also revealed to play important roles in characterizing dynamics for densities on a continuous space, e.g., Gaussian convolution, diffusion processes, and FPE\cite{53–55}. Various governing equations in physics were claimed to be derived in a unified way from this quantity\cite{35}. The quantity $\mathbb{I}_F$ looks like the Fisher information\cite{56} but is different from the conventional Fisher information matrix \cite{57–59} because the derivative $\nabla r \ln p(r)$ is not for the parameters but for the base space variable of $p(r)^{[2]}$. Because $\mathbb{I}_F$ is a scalar, we follow \cite{58} and call it Fisher information number. The Fisher information number $\mathbb{I}_F$ was found to be related to the Kullback-Leibler divergence in additive Gaussian channels\cite{53} and other

\footnote{The relation between the two forms of Fisher information has been explained in multiple ways. For example, they are related as the shift of the base space via parameters\cite{35, 60}. The Fisher information number was introduced by Rao\cite{57}.}
systems[55, 61], which is known as the De Bruijn identity[53]. In addition, the logarithmic Sobolev inequality is also viewed as a relation between the Fisher information number and the KL divergence (or Shannon information)[62, 63]. These results have recently been associated with the formal Riemannian geometric structure induced by the $L^2$-Wasserstein geometry[64, 65].

C. Information geometry and dynamics in machine learning

On top of these traditional trends, information geometry is now playing pivotal roles in machine learning to design and evaluate online optimization algorithms (dynamics) in the space of model parameters such as natural gradient[66] and mirror descent[67, 68] as well as evolutionary computation (information-geometric optimization) [69]. Geometric interpretation allows us to understand the behaviors and efficiency of algorithms and their dynamics more intuitively in a principled manner[68–70].

D. Aim and contributions of this work

Despite the wide applicability and the history of information geometry, we still lack a solid theoretical framework to unify these outcomes that spread across different fields from the viewpoint of information geometry. In this work, we introduce a new information geometric structure for the dynamics of probability and positive densities. In this structure, we consider not only the single dually flat structure built on the space of densities as in [23, 24] but also another structure constructed on the space of fluxes. The two of them are linked algebraically and topologically via the continuity equation and the gradient equation as illustrated in Fig. 1.

Under this doubly dual flat structure, we can consider the dynamics of densities as a generalized flow, and various results known so far can be unified in this framework. We exclusively consider dynamics of densities on finite-dimensional discrete manifolds, i.e., finite graphs or hypergraphs, because the structure introduced here can be explicitly manifested in this setup and also because we do not need the mathematically elaborated setup for infinite-dimensional information geometry on a smooth manifold[71]. For the case of FPE in a continuous state space, the dually flat structure built on the flux space is reduced to
the formal Riemannian geometric structure of $L^2$ Wasserstein geometry because the convex functions that induce the dually flat structure become quadratic. Our structure generalizes the linear inner product on the tangent and cotangent spaces of the Riemannian structure with the nonlinear Legendre transform, thereby requiring information and Hessian geometry. By elucidating this information geometric structure, we can easily see that some quantities such as the bilinear product, convex thermodynamic potential functions, the Fisher information matrix, and the Fisher information number are consolidated into one quantity for FPE with the quadratic convex functions (see Sec. V D and Sec. V E). Therefore, our structure provides a way to unify the dualistic gradient flow mentioned in Sec. IA and also the information-number related topics in Sec. IB.

From the viewpoint of homological algebra, the structure we work on is a modification of the chain and cochain complexes of graphs or hypergraphs by replacing the usual inner product duality[72] on each pair of chains and cochains with Legendre duality. Moreover, the dually flat space built on the flux space is linked to a finite-dimensional version of Orlicz spaces[73], which have been employed for constructing infinite-dimensional information geometry[71]. From this generalization and the nice properties of the doubly dual flat structures, we can obtain generalized versions of the Helmholtz-Hodge-Kodaira (HHK) de-

FIG. 1. Diagrammatic illustration of the doubly dual flat structure established on the vertex spaces (left) and edge spaces (right), which are topologically related via the underlying graph or hypergraph.
composition (Thm. 1), the Otto calculus (Thm. 2), and its extension to cycle spaces (Thm. 3).

Our construction of information geometry for dynamics is heavily based on the idea of using Legendre duality for the force and flux relation, proposed in the recent work of large deviation theory and macroscopic fluctuation theorem for MJP and CRN led by A. Mieleke, R.I.A. Petterson, M.A. Peletier, D.R.M. Renger, J. Zimmer, and others\cite{3, 74–81}. We clarified its information-geometric aspects in the context of CRN and thermodynamics in our previous work\cite{82}. We also concurrently elucidated the intimate link of equilibrium chemical thermodynamics and information geometry on the density state space \cite{83–85}. In light of those, the contribution of this work is three-fold. First, we integrate these results in terms of information geometry, which clarifies the underlying geometric nature of the problem, provides transparent interpretations for known results, and leads to new information geometric results and insights (Thm. 1–Thm. 3); Second, this structure substantially extends the applicability of information geometry to a wide variety of dynamical problems and can unify the results obtained in different disciplines; Lastly, the structure links information geometry to algebraic graph theory, discrete calculus, and algebraic homology, which was not appreciated before and provides a way to consider the topology of the underlying manifold in information geometry.

E. Organization of this paper

This work is organized as follows: In Sec. II, we introduce the models of dynamics on graphs and hypergraphs. In Sec. III, we outline the homological algebra of graphs and hypergraphs. In Sec. IV, we abstractly introduce the doubly dual flat structures on the density and flux spaces and define the generalized flow associated with the structures. In Sec. V, we clarify that the introduced structures include a wide class of dynamics on graph and hypergraph. In Sec. VI and Sec. VII, we further define information-geometric objects and quantities, which naturally appear from the setup and play an integral role in the subsequent analysis of dynamics. In Sec. VIII and Sec. IX, we derive several results for equilibrium and nonequilibrium flows, respectively. Finally, we provide a summary and prospects of our work in Sec. X. The notation and symbols are listed in Appendix.

\cite{3} Ordered alphabetically.
II. CLASSES OF MODELS FOR DYNAMICS ON GRAPH AND HYPERGRAPH

In this work, we focus on linear and nonlinear dynamics defined on graphs[86] and hypergraphs[87].

The linear dynamics on graphs (LDG) includes Markov jump processes (MJP)[88], consensus dynamics[89], monomolecular chemical reaction networks[90], linear electric circuits [91], and other linear dynamics on graphs[86, 92]. We consider an extension of LDG to hypergraphs and nonlinear dynamics, common instances of which are chemical reaction networks (CRN) with the law of mass action (LMA) kinetics [8] and polynomial dynamical systems (PDS)[93]. Because the extension we deal with in this work is a subclass of nonlinear dynamical systems on hypergraphs, we use CRN to designate this subclass.

In the following subsections, LDG and CRN are introduced using the language of algebraic graph theory[86, 94]. Then, we also give a brief and formal introduction of the Fokker-Planck equation (FPE)[3], a linear dynamics of the probability density defined in Euclidean space. We use the FPE throughout this paper to contrast our results with the previous ones obtained for FPE.

A. Reversible Linear Dynamics on Graph

**Definition 1** (Edge-weighted finite graph \(G_{k^\pm}\)). A finite graph \(G := (\{v_i\}, \{e_e\}, B)\) consists of \(N_v\) vertices, \(\{v_i\}_{i \in [1,N_v]}\), and \(N_e\) oriented edges \(\{e_e\}_{e \in [1,N_e]}\), each of which connects two different vertices\[4\] (Fig. 2 (a)). The incidence relation is represented by the incidence matrix \(B \in \{0, \pm 1\}^{N_v \times N_e}\) where, for \(B = (b_{i,e})\),

\[
\begin{align*}
    b_{i,e} := +1 & \quad \text{if } v_i \text{ is the head of edge } e_e, \\
    b_{i,e} := -1 & \quad \text{if } v_i \text{ is the tail of edge } e_e, \\
    b_{i,e} := 0 & \quad \text{otherwise.}
\end{align*}
\]

An edge-weighted finite graph \(G_{k^\pm} := (\{v_i\}, \{e_e\}, B, \{k_e^\pm\})\) has two positive weighting parameters \(k_e^\pm = (k_e^+, k_e^-) \in \mathbb{R}_{>0}\) for each edge \(e_e\). Parameters \(k_e^+\) and \(k_e^-\) are denoted as forward and reverse rates or weights of the edge \(e\), respectively.

\[4\] This means that we exclude loops.
A reversible linear dynamics (rLDG) on a graph is defined on the edge-weighted finite graph $G_{k^\pm}$:

**Definition 2** (Reversible linear dynamics on a graph $G_{k^\pm}$). The reversible linear dynamics of the non-negative density $\mathbf{x}(t) = (x_1(t), \ldots, x_{N_v}(t))^T \in \mathbb{R}_{\geq 0}^{N_v}$ on $G_{k^\pm}$ is defined by the continuity equation

$$\dot{\mathbf{x}} = -\mathbb{B} \mathbf{j}(\mathbf{x}) = -\mathbb{B} [\mathbf{j}^+(\mathbf{x}) - \mathbf{j}^-(\mathbf{x})], \quad (2)$$

and linear forward and reverse one-way fluxes $\mathbf{j}^\pm(\mathbf{x}) = (j_1^\pm(\mathbf{x}), \ldots, j_{N_e}^\pm(\mathbf{x}))^T \in \mathbb{R}_{\geq 0}^{N_e}$ with the following specific functional form$^5$:

$$\mathbf{j}^\pm(\mathbf{x}) = \mathbf{k}^\pm \circ (\mathbb{B}^\pm)^T \mathbf{x}, \quad (3)$$

where $\mathbf{j}(\mathbf{x}) := \mathbf{j}^+(\mathbf{x}) - \mathbf{j}^-(\mathbf{x})$ is the total flux, the symbol $\circ$ denotes the component-wise product of two vectors$^6$, and $\mathbb{B}^+$ and $\mathbb{B}^-$ are the head and tail incidence matrices defined respectively as $\mathbb{B}^+ := \max[\mathbb{B}, 0]$ and $\mathbb{B}^- := \max[-\mathbb{B}, 0]$. The incidence matrix $\mathbb{B}$ in Eq. 2 is often regarded as the discrete divergence operator on a graph$^7$ and denoted also as

$^5$ We may consider other functional forms for $\mathbf{j}(\mathbf{x})$, which can induce nonlinear dynamics on the graph. In this work, we focus mainly on the linear case.

$^6$ Also known as the Hadamard product or Schur product of vectors.
A reversible Markov jump process (rMJP) is a representative class of the rLDG describing random jumps of noninteracting particles on $G_{k^\pm}$. The weighting parameter $k_e^+$ is interpreted as the forward jump rate from the head of the oriented edge $e$ to its tail, whereas $k_e^-$ is the reverse jump rate from the tail to the head of $e$.[8] For infinitely many such particles, we consider $p_i(t) \in [0, 1]$, the fraction of particles on vertex $v_i$ at time $t$, which is a non-negative density on vertices. Then, the forward and reverse one-way fluxes on the $e$th edge defined by Eq. 3 are represented as

$$j_e^+(p) = k_e^+ p_{v_e^+} \in \mathbb{R}_{\geq 0}, \quad j_e^-(p) = k_e^- p_{v_e^-} \in \mathbb{R}_{\geq 0},$$

(4)

where $v_e^+$ and $v_e^-$ are the head and tail vertices of edge $e$.[9] The linearity of $j_e^+(p)$ with respect to $p$ comes from the independence of the dynamics of each particle on the graph. Then, the continuity equation (Eq. 2) with the state vector $p(t):=(p_1(t), \ldots, p_{N_v}(t))^T \in \mathbb{R}_{\geq 0}^{N_v}$ is reduced to the master equation: $\dot{p} = -B j(p)$.

**Definition 3** (Weighted asymmetric graph Laplacian[94, 95]). For $G_{k^\pm}$, the corresponding weighted asymmetric graph Laplacian is defined by

$$L_{\theta} := B \left[ \text{diag} [k^+] (B^+)^T - \text{diag} [k^-] (B^-)^T \right],$$

(5)

where $\theta := (k^+, k^-)$. Using $L_{\theta}$, Eq. 2 and Eq. 3 are represented as

$$\dot{x} = -B j(x) = -B \left[ \text{diag} [k^+] (B^+)^T - \text{diag} [k^-] (B^-)^T \right] x = -L_{\theta} x.$$ 

(6)

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[7] This interpretation is because Eq. 2 is associated with the continuity equation on a Euclidean space or on a Riemannian manifold where we have the divergence operator $\nabla \cdot$ instead of $B$. However, divergence on a Riemannian manifold implicitly includes the information of the metric via the Hodge operator. On the contrary, $B$ does not. From the viewpoint of homology algebra, $B$ should be regarded as the adjoint (transpose) of the discrete exterior derivative operator $\delta^0 := B^T$, which is also often called a discrete gradient operator[72]. For a Euclidean space, they are the same.

[8] If we allow $k_e^\pm$ to be 0, we can include the irreversible MJP and also LDG in this formulation. We leave this extension for future work because it should require additional assumptions on the Legendre duality introduced in the subsequent sections.

[9] Here, we have abused the notation $v_e^+$ to indicate the index of the vertex $v_e^+$ of $e$ only when $i$ is the index of the head (tail) vertex $v_e^+$ of $e$ and 0 otherwise.
The operator $\mathcal{L}_\theta$ is reduced to the weighted symmetric graph Laplacian if $k^+ = k^-$ and also to the conventional graph Laplacian if $k^+ = k^- = 1$ [94, 95]. Eq. 6 can cover linear transport on graphs, consensus dynamics on graphs [89], and other linear dynamics on graphs [86, 92].

B. Chemical reaction network and polynomial dynamics on hypergraphs

Next, we introduce a class of nonlinear dynamical systems on hypergraphs, which includes the rLDG (Eq. 2 and Eq. 3) as a special case. The most common instance is deterministic chemical reaction networks (CRN) with the law of mass action (LMA) kinetics [7, 8, 44, 96], and this class is sometimes referred to as polynomial dynamical systems (PDS). Because the major part of the PDS theory has been developed for CRN, we use CRN to introduce and specify this class of nonlinear systems in this work.

**Definition 4** (Reversible CRN hypergraph). The reversible CRN hypergraph $H := (\{X_i\}_{i \in [1,N_X]}, \{e_e\}_{e \in [1,N_e]}, \mathbb{L}, \mathbb{B})$ consists of a finite number of vertices $\{X_i\}_{i \in [1,N_X]}$ and hyperedges $\{e_e\}_{e \in [1,N_e]}$ where $N_X, N_e \in \mathbb{Z}_{>0}$ (Fig. 2 (b)). Each hyperedge $e_e$ connects two different hypervertices $\hat{v}_e^+$ and $\hat{v}_e^-$ where $\hat{v}_e^+ \neq \hat{v}_e^-$[10]. The hypervertices are multisets of vertices $\{X_i\}_{i \in [1,N_X]}$, each of which is defined as $\hat{v}_\ell = \sum_{i=1}^{N_X} \gamma_{i,\ell} X_i$ where $\gamma_{i,\ell} \in \mathbb{Z}_{\geq 0}$ is the number of the $i$th vertex included in the $\ell$th hypervertex. Thus, the nonnegative integer vector $\hat{\gamma}_\ell := (\gamma_{1,\ell}, \cdots, \gamma_{N_X,\ell})^T \in \mathbb{Z}_{\geq 0}^{N_X}$ defines the $\ell$th hypervertex. Let $N_\hat{v}$ be the total number of the hypervertices and $\mathbb{L} := (\gamma_1, \cdots, \gamma_{N_\hat{v}}) \in \mathbb{Z}_{\geq 0}^{N_\hat{v} \times N_\hat{v}}$ be the hypervertex matrix. The matrix $\mathbb{B} \in \{0, \pm\}^{N_\hat{v} \times N_\hat{v}}$ is the incidence matrix encoding the incidence relations among the hypervertices and the hyperedges. The hypergraph incidence matrix $S \in \mathbb{Z}^{N_\hat{v} \times N_\hat{e}}$ is then defined as

$$S := \mathbb{L} \mathbb{B}.$$

If $\mathbb{L} = I$ where $I$ is the identity matrix, then $H = (\{X_i\}_{i \in [1,N_X]}, \{e_e\}_{e \in [1,N_e]}, I, \mathbb{B})$ is reduced to $\mathcal{G} = (\{\hat{v}_\ell\}_{\ell \in [1,N_\hat{v}]}, \{e_e\}_{e \in [1,N_e]}, \mathbb{B})$ where $\hat{v}_\ell = X_\ell$.

In the context of CRN theory, the vertices $\{X_i\}$ correspond to the molecular species involved in a CRN, and each hyperedge $e_e$ represents a pair of forward and reverse reactions:

$$\gamma_{1,e}X_1 + \cdots + \gamma_{N_X,e}X_{N_X} \Rightarrow \gamma_{1,e}X_1 + \cdots + \gamma_{N_X,e}X_{N_X},$$

[10] This means that we exclude loop hyperedges.
where the forward and reverse reactions are from left to right and from right to left, respectively. Head and tail hypervertices \( \hat{v}_e^+ := (\gamma_1^+ \mathcal{X}_1 + \cdots + \gamma_{N_e}^+ \mathcal{X}_{N_e}) \) and \( \hat{v}_e^- := (\gamma_1^- \mathcal{X}_1 + \cdots + \gamma_{N_e}^- \mathcal{X}_{N_e}) \) in Eq. 8 are the sets of reactants and products of the \( e \)th forward reaction, respectively. More specifically, \( \gamma_{i,e}^+ \in \mathbb{Z} \) and \( \gamma_{i,e}^- \in \mathbb{Z} \) are the numbers of the molecules \( \mathcal{X}_i \) involved as the reactants and products of the \( e \)th forward reaction, respectively. For the reverse reaction, \( \hat{v}_e^- \) and \( \hat{v}_e^+ \) are the reactants and products. The hypervertices are called complexes in CRN theory \([8][11]\). From \( \{\gamma_{i,e}^+\} \) and \( \{\gamma_{i,e}^-\} \), we can define \( s_e := (\gamma_{1,e}^+ - \gamma_{1,e}^-, \cdots, \gamma_{N,e}^+ - \gamma_{N,e}^-)^T \in \mathbb{Z}^{N_e} \), \( (9) \)

where \( \mp s_e \) specify the change in the number of molecules induced when the \( e \)th forward or reverse reaction occurs just once, respectively. The hypergraph incidence matrix \( S \) defined in Eq. 7 is represented as \( S = (s_1, \cdots, s_{N_e}) \in \mathbb{Z}^{N_e \times N_e} \). In chemistry, the negative of \( s_e \) and \( S \), i.e., \(-s_e \) and \(-S\), are called the stoichiometric vector and matrix, respectively\([8]\).

**Remark 1.** To define a reversible CRN hypergraph, the hypergraph matrix \( S \) is not sufficient. If the head and tail hypervertices of a hyperedge can contain the same vertex (molecule), the corresponding element in \( S \) of such a shared vertex becomes 0 by canceling out. Thus, the existence of shared vertices (molecules) is invisible in \( S \), and the pair \((\mathcal{L}, \mathcal{B})\) is required to define \( H \). Such shared molecules are called catalysts in CRN.

For a CRN hypergraph, the continuity equation for CRN is defined:

**Definition 5** (CRN continuity equation). Let a vector of nonnegative densities \( x = (x_1, \cdots, x_{N_e})^T \in \mathbb{R}_{\geq 0}^{N_e} \) represents the concentration of molecules \( \{\mathcal{X}_i\} \). The CRN continuity equation is defined as

\[
\dot{x} = -Sj(x) = -\text{div}_S j(x),
\]

where \( j^+_e(x) \in \mathbb{R}_{\geq 0} \) and \( j^-_e(x) \in \mathbb{R}_{\geq 0} \) are the one-way fluxes of the \( e \)th forward and reverse reactions, \( j^±_e(x) := (j^+_1(x), \cdots, j^+_N(x))^T \in \mathbb{R}_{\geq 0}^{N_e} \) are their vector representations, and \( j(x) := j^+_e(x) - j^-_e(x) \in \mathbb{R}^{N_e} \) is the total reaction flux\([7, 8, 96]\). The hypergraph divergence operator \( \text{div}_S := S \) is defined accordingly.

\[\text{[11]}\] Because we use the term complex to for the cell complex in homological algebra, we use hypervertices to indicate the complexes of the CRN theory.
To define the dynamics of a CRN, the functional form of $j^\pm_e(x)$ is required\[12\]. Before introducing specific forms, we define two important properties of the flux and also other functions defined on edges:

**Definition 6** (Consistency of the flux $j^\pm(x)$ with the hypergraph $H$). The one-way flux $j^\pm(x)$ is consistent with the hypergraph $H$ if, for all $e \in [1, N_e]$, $j^\pm_e(x)$ becomes 0 when $x_i = 0$ where $x_i$ is any reactant of $j^\pm_e(x)$, respectively. In other words, $j^\pm_e(x)$ satisfies

$$\gamma^\pm_{i,e}j^\pm_e(x) = 0 \text{ if } x_i = 0 \text{ for any } i \in [1, N_X].$$

**Definition 7** (Locality of function on edges over $H$). A vector function $g(x) \in \mathbb{R}^{N_e}$ defined on the edges is local on $H$ if, for all $e \in [1, N_e]$, $g_e(x)$ is a function only of the elements of $x$ incident to the edge $e$ on $H$, i.e., $g_e(x) = g_e(\gamma^+_{1,e}x_1, \cdots, \gamma^+_{N_X,e}x_{N_X}, \gamma^-_{1,e}x_1, \cdots, \gamma^-_{N_X,e}x_{N_X})$ where $\gamma^\pm_{i,e} := \min[1, \gamma^\pm_{i,e}] \in \{0, 1\}$.

The consistency condition is indispensable to prohibit a reaction that can decrease $x_i$ from occurring when $x_i = 0$. For $j^\pm(x)$, the locality means that the flux of the $e$th reaction depends only on the concentrations of its reactants and products. The local flux is determined solely by the information stored on the vertices incident to the edge and plays a crucial role when we regard the structure introduced in this work as an extension of differential forms on continuous manifolds to graphs and hypergraphs. When we work on specific forms of fluxes, we consider only local fluxes consistent with the given hypergraph $H$.

In chemistry, we have a variety of candidates for the functional form of flux, e.g., the Michaelis-Menten function, Hill’s function, and others\[7, 97\]. Among those, the LMA kinetics is the most basic and well-established one.

**Definition 8** (Waage-Guldberg’s law of mass action kinetics (LMA kinetics)). A CRN follows the LMA kinetics if, for all $e \in [1, N_e]$, the $e$th forward and reverse reaction fluxes are represented as

$$j^\pm_e(x) = k^\pm_e \prod_{j=1}^{N_X} x_j^{\gamma^\pm_{j,e}} = k^\pm_e \sum_{\ell=1}^{N_e} \prod_{j=1}^{N_X} x_j^{\gamma^\pm_{j,\ell}} = b^\pm_e \prod_{j=1}^{N_X} x_j^{\gamma^\pm_{j,e}},$$

Even though the functional form of $j^\pm_e(x)$ is automatically determined in the case of LDG because of the linearity, we have multiple possibilities to define $j^\pm_e(x)$ for the nonlinear case.
where $k_e^+ \in \mathbb{R}_{>0}$ and $k_e^- \in \mathbb{R}_{>0}$ are the reaction rate constants of the $e$th forward and reverse reactions, respectively. In this form, it can be compactly represented as

$$j_{MA}^\pm (x) = k^\pm \circ (B^\pm)^T x^L_T,$$

where $x^\gamma := \prod_{j=1}^{N_x} x_j^\gamma_j \in \mathbb{R}_{\geq 0}$ and $x^L_T := (x^\gamma_1, \ldots, x^\gamma_{N_x})^T \in \mathbb{R}_{\geq 0}^{N_x}$.[13] We use the subscript MA as in $j_{MA}^\pm (x)$ to discriminate this specific form of the flux from others. We can easily observe that $j_{MA}^\pm (x)$ is consistent and local with respect to $H$.

**Remark 2 (Algebraic aspect of LMA kinetics).** Because $x^L_T$ is a vector of monomials of $x$, each one-way flux, $j_e^+(x)$ and $j_e^-(x)$ are monomials of $x$ under Eq. 12 and thus the total flux $j_e(x) = j_e^+(x) - j_e^-(x)$ is a binomial. This fact links the real algebraic geometry of the toric varieties[98, 99] to CRN[100, 101] as it does in algebraic statistics[102, 103].

**Remark 3 (Extended LMA kinetics).** While we mainly work on the normal LMA kinetics, we can extend it. The extended LMA kinetics defined on $H$ is defined as

$$j_{eMA}^\pm (x) = k^\pm \circ g(x) \circ (B^\pm)^T x^L_T,$$

where $g(x) \in \mathbb{R}_{>0}^{N_e}$ for $x \in \mathbb{R}_{\geq 0}^{N_x}$ and is local with respect to $H$.[14] An example of the extended LMA kinetics is reversible Michaelis-Menten kinetics[105].

By combining the continuity equation (Eq. 10) and the LMA kinetics (Eq. 12), we have the following:

$$\dot{x} = -S j_{MA}(x) = -L_B \left[ \text{diag}[k^+](B^+)^T - \text{diag}[k^-](B^-)^T \right] x^L_T = -L_\theta x^L_T,$$

where $L_\theta$ is the weighted asymmetric graph Laplacian defined as in Eq. 5. Now, we can see that CRN contains rLDG (Eq. 6) as a special case if $L = I$. Owing to this inclusion relation, there exists another type of extension known as generalized LMA kinetics where the monomials $x^L_T$ are replaced with fractional monomials, i.e., powers of $x$ with nonnegative real-valued exponents[104].

[13] We should note an important relation,[14] which holds because every column vector of $B^\pm$ contains only one +1 and the others are 0.
CRN with LMA kinetics is a mathematically sound generalization of rLDG. Because LDG has been used in various fields of social science, network science, machine learning, and so on, CRN theory is potentially important for extending the results there.

C. Fokker Planck Equations

While our main focus is the dynamics on graphs and hypergraphs, we use the FPE as a representative class of dynamics on a continuous Euclidean state space. Specifically, we use FPE only to demonstrate the relation of our results with previous ones obtained for FPE in various contexts. Because FPE is infinite-dimensional, we treat it here only formally.

Let \( r \in \mathbb{R}^d \) be a vector in a \( d \) dimensional Euclidean space. We consider infinitely many noninteracting particles randomly walking in the space and describe the dynamics by a probability density \( p_t(r) \) of the particles. The continuity equation for \( p_t(r) \in \mathbb{R}_{\geq 0} \) is

\[
\partial_t p_t(r) = -\nabla \cdot \mathbf{j}_{FP}[p_t(r)] \tag{15}
\]

where \( \mathbf{j}_{FP}[p_t(r)] \in \mathbb{R}^d \) is the probability flux, \( \nabla := (\partial/\partial r_1, \cdots, \partial/\partial r_d)^T \) is the gradient operator on the Euclidean space, and \( (\nabla \cdot) : \nabla \cdot \mathbf{F}(r) := \sum_{i=1}^{d} \partial F_i(r)/\partial r_i \in \mathbb{R} \) is the divergence. The flux of the FPE is defined as

\[
\mathbf{j}_{FP}[p(r)] = [\mathbf{F}(r)p(r) - D_0 \nabla p(r)] , \tag{16}
\]

where \( \mathbf{F}(r) \in \mathbb{R}^d \) is the drift force, \( D_0 \in \mathbb{R}_{>0} \) is the diffusion constant.

III. DISCRETE CALCULUS AND HOMOLOGICAL ALGEBRA OF GRAPHS AND HYPERGRAPHS

The algebraic and topological structure of the dynamics on graphs and hypergraphs can be explicitly and abstractly treated by using the language of discrete calculus and homological algebra. The discrete version of the gradient and divergence mentioned in Sec. II is also characterized. In this section, we briefly introduce the chain and cochain complexes defined for a finite graph or a hypergraph and discrete calculus[72, 94, 106, 107]. We first introduce the complexes for a graph \( \mathcal{G} \) and then extend them to a hypergraph \( \mathcal{H} \) algebraically[15].

[15] The complex used here should not be confused with complexes used in CRN theory[8].
should be noted that the conventional discrete calculus (the discrete version of the theory for differential forms) presumes the metric structure in the dual space of chains and cochains or that of cochains on primal and dual complexes \[108, 109\]. However, we are going to introduce Legendre duality instead. For this purpose, our introduction of chain and cochain complexes depends only on the topological (algebraic) information of the underlying graph and hypergraph[72] without specifying the metric information.

A. Chain and cochain complexes on graphs

The elements of a graph \(G\) are called cells in discrete calculus and algebraic graph theory \[16\]. A vertex and an edge are, respectively, called 0-cell and 1-cell, and the graph \(G\) is denoted as a cell-complex\[17\]. For each type of cell, we consider vectors (chains and cochains) defined on the cells. For \(G\), a 0-chain with field \(\mathbb{R}\) is an \(N_v\)-tuple of real scalars, each of which is assigned to a vertex, i.e., a 0 cell. Thus, a 0-chain is a real vector defined on the vertices of \(G\) with the basis \(\{v_i\}\). This basis is called the standard basis. The components of the vector \(x \in C_0(G)\) are given as \(x(v_i) := x_i\). The vector space of real 0-chains is called the vertex space and denoted as \(C_0(G) = \mathbb{R}^{N_v}[18][19]\). Similarly, a real 1-chain is a real vector defined on the edges of \(G\). The real vector space of 1-chains is called the edge space and denoted as 

\[16\] We follow the terminology in [72]. While we use \[18\] In algebraic graph theory, the chain of a graph \(G\) is defined as an integer-valued vector space \(\mathbb{Z}^{N_v}\) to represent the discrete and combinatorial nature of \(G\) and also to specify the domain of integration. Here, we use \(\mathbb{R}\) as the field of the vector space. Specifically, our chains \(C_p(G; \mathbb{R})\) should be considered as the cochains on the dual complex \(C^p(G^*; \mathbb{R})\), which is isomorphic to \(C_p(G; \mathbb{R})\). In the theory of differential forms on \(N\)-dimensional manifolds, \(p\)-forms (\(p\) cochains) and \((N - p)\)-forms (\(N - p\) cochains) have the same dimension. The \(p\)-form and the \((N - p)\)-form are linked by the Hodge star operator. For a cell complex, this duality be-
$C_1(\mathcal{G}) = \mathbb{R}^{N_*}$. The standard basis is introduced by using edges $\{e_i\}$ accordingly. A flux $j$ is a 1-chain: $j(e_i) := j_i[20]$. The graph incidence matrix $\mathcal{B}$ induces the discrete differential $\delta_1 : C_1(\mathcal{G}) \to C_0(\mathcal{G})$ as $\delta_1 j := \mathcal{B} j[21]$.

To obtain an exact sequence, we algebraically define the $(-1)$ and 2 chains and the corresponding differentials $\delta_0$ and $\delta_2$. Let $C_2(\mathcal{G}) = \mathbb{R}^{N_z}$ where $N_z = \dim[\text{Ker}\mathcal{B}]$ and $\{v_i\}_{i \in [1,N_z]}$ is a set of complete basis of $\text{Ker}\mathcal{B}$ where $v_i \in \{0, +1, -1\}^{N_*}$. In algebraic graph theory, $\text{Ker}\mathcal{B}$ is called a cycle subspace[86, 94, 110]. For a graph $\mathcal{G}$, we can construct $\{v_i\}_{i \in [1,N_z]}$ by, for example, using the fundamental cycle basis of $\mathcal{G}$ obtained from a fixed spanning tree of $\mathcal{G}$[22][86]. Thus, $C_2(\mathcal{G})$ is the vector space defined on the cycles of $\mathcal{G}$ and isomorphic to the cycle subspace. We define a matrix, $\forall := (v_1, \cdots, v_{N_z})[23]$, and the differential $\delta_2 : C_2(\mathcal{G}) \to C_1(\mathcal{G})$ as $\delta_2 := \forall$. From the construction, $\mathcal{B} \forall = \delta_1 \delta_2 = 0$ and $\text{Im}[\delta_2] = \text{Ker}[\delta_1]$ hold. Similarly, let $C_{-1}(\mathcal{G}) = \mathbb{R}^{N_l}$ where $N_l = \dim[\text{Ker}\mathcal{B}^T]$ and $\{u_{i,\ell}\}_{\ell \in [1,N_l]}$ is a set of complete basis of $\text{Ker}\mathcal{B}^T$ where $u_{i,\ell} \in \{0, +1, -1\}^{N_*}$. The subspace $\text{Ker}\mathcal{B}^T$ is related to the connected components of $\mathcal{G}$ and $u_i$ can be chosen such that $u_{i,\ell} = +1$ if the $i$th vertex is included in the $\ell$th connected component. Thus, $C_{-1}(\mathcal{G})$ is the vector space on the connected components. From the matrix $\forall := (u_1, \cdots, u_{N_l})^T$, the differential $\delta_0 : C_0(\mathcal{G}) \to C_{-1}(\mathcal{G})$ is defined as $\delta_0 := \forall$. From the construction, $\mathcal{B} \forall = \delta_0 \delta_1 = 0$ and $\text{Im}[\delta_1] = \text{Ker}[\delta_0]$ hold. Then, we obtain

Between $p$- and $(N - p)$-forms is algebraically represented by the dual complex. For a graph, the 0-cochain of the dual complex is isomorphic to the 0-chain of the complex[72]. Here, to make the presentation simple without introducing the dual complex, we avoid these technical arguments.

In the theory of differential forms, the density is an $N$-form (cochain) of an $N$ dimensional manifold, which is linked to a 0-form via the Hodge star operator.

Again, in the theory of differential forms, the flux is an $(N - 1)$-form (cochain) of an $N$ dimensional manifold. Through the Hodge star operator, we identify it with the 1-chain with the field $\mathbb{R}$.

In algebraic graph theory, $\mathcal{B}$ is also identical to the discrete boundary operator from $C_1(\mathcal{G}; \mathbb{Z})$ to $C_0(\mathcal{G}; \mathbb{Z})$.

The spanning tree chosen defines a fundamental cycle and cocycle bases.

$\forall^T$ is called the fundamental tieset matrix in graph theory.
the exact chain sequence\textsuperscript{[24][25]}:
\begin{equation}
0 \leftarrow C_{-1}(\mathcal{G}) \xleftarrow{\delta_{-1}=U} C_0(\mathcal{G}) \xleftarrow{\delta_1=E} C_1(\mathcal{G}) \xleftarrow{\delta_2=V} C_2(\mathcal{G}) \leftarrow 0. \tag{17}
\end{equation}

Because $C_p(\mathcal{G})$ is a vector space for each $p = \{-1, 0, 1, 2\}$, we can consider its dual vector space $C^p(\mathcal{G}) := C^*_p(\mathcal{G})$ consisting of the linear functions on $C_p(\mathcal{G})$. An element of $C^p(\mathcal{G})$ is called $p$-cochain. Let $\langle \cdot, \cdot \rangle : C_p(\mathcal{G}) \times C^p(\mathcal{G}) \rightarrow \mathbb{R}$ be the standard bilinear pairing of the $p$-chain and $p$-cochain defined with the standard basis. The transposes of $U$, $B$, and $V$ induce the differentials between cochains as

$\delta^{-1} := U^T : C^{-1}(\mathcal{G}) \rightarrow C^0(\mathcal{G})$, $\delta^{0} := B^T : C^0(\mathcal{G}) \rightarrow C^1(\mathcal{G})$, and $\delta^{1} := V^T : C^1(\mathcal{G}) \rightarrow C^2(\mathcal{G})$. The differentials $\delta^p$ on cochains are the adjoint of the differentials $\delta_p$ on chains, which induce the exact cochain sequence:
\begin{equation}
0 \rightarrow C^{-1}(\mathcal{G}) \xrightarrow{\delta^{-1}=U^T} C^0(\mathcal{G}) \xrightarrow{\delta^{0}=B^T} C^1(\mathcal{G}) \xrightarrow{\delta^{1}=V^T} C^2(\mathcal{G}) \rightarrow 0. \tag{18}
\end{equation}

Note that the definition of chains, cochains, and differential operators are topological in the sense that we do not include any metric information in them.

\section*{B. Chain and cochain complexes on hypergraphs}

The definitions of chain and cochain complexes introduced above are algebraically extended to hypergraphs $\mathcal{H}$ simply by replacing the graph incidence matrix $\mathcal{B}$ with the hypergraph incidence matrix $\mathcal{S}$.

\textbf{Definition 9} (Exact chain and cochain sequences on a hypergraph). The chain and cochain complexes on a hypergraph are defined by the following diagram:

\begin{equation}
\begin{array}{cccc}
0 & \rightarrow & C^{-1}(\mathcal{H}) & \xrightarrow{\delta^{-1}=U^\mathcal{H}} C^0(\mathcal{H}) & \xrightarrow{\delta^{0}=S^\mathcal{H}} C^1(\mathcal{H}) & \xrightarrow{\delta^{1}=V^\mathcal{H}} C^2(\mathcal{H}) & \rightarrow 0 \\
0 & \leftarrow & C_{-1}(\mathcal{H}) & \xleftarrow{\delta_{-1}=U} C_0(\mathcal{H}) & \xleftarrow{\delta_1=S} C_1(\mathcal{H}) & \xleftarrow{\delta_2=V} C_2(\mathcal{H}) & \leftarrow 0.
\end{array}
\end{equation}

where $C^{-1}(\mathcal{H}) = C_{-1}(\mathcal{H}) = \mathbb{R}^N$, $C^0(\mathcal{H}) = C_0(\mathcal{H}) = \mathbb{R}^{N_x}$, $C^1(\mathcal{H}) = C_1(\mathcal{H}) = \mathbb{R}^{N_e}$, and $C^2(\mathcal{H}) = C_2(\mathcal{H}) = \mathbb{R}^{N_z}$.

\textsuperscript{[24]} We should note that the sequence is not canonical \textsuperscript{[25]} Upon necessity, we can consider the harmonic components by employing an under-complete basis for $V$. because $U$ and $V$ depend on the choice of bases.
The bases, $V$ and $U$, are obtained as integral bases, i.e., the components of $V$ and $U$ can be chosen from $\mathbb{Z}$ because $S$ is an integer-valued matrix\textsuperscript{26}. As we will explain in Sec. VI and Sec. IX, the meaning of $C_2(\mathbb{H})$ can be retained as the space on generalized cycles. The meaning of $C_{-1}(\mathbb{H})$ becomes the space of conserved quantities under the dynamics (Eq. 10).

C. Discrete calculus on graphs and hypergraphs

The $p$-cochain and $p$-chain introduced above are the algebraic abstraction of the $p$-differential form and its Hodge dual on a differential manifold\textsuperscript{72}. Accordingly, the discrete versions of gradient, divergence, and curl are associated with the differentials (exterior derivative).

**Definition 10** (Discrete gradients, divergences, and curls). The discrete gradient is defined as $\text{grad}_B := \delta^0 = B^T$ for $G$ and also as $\text{grad}_S := \delta^0 = S^T$ for $H$. The adjoints of the gradients are defined with the corresponding adjoint differentials: $\text{grad}^*_B := \delta_1 = B$ and $\text{grad}^*_S := \delta_1 = S$. They are called discrete divergences and denoted as $\text{div}_B = \text{grad}^*_B$ and $\text{div}_S = \text{grad}^*_S$\textsuperscript{27}\textsuperscript{28}\textsuperscript{29}. The discrete curl and its adjoint are defined as $\text{curl}_V := \delta^1 = V^T$ and $\text{curl}^*_V := \delta_2 = V$, respectively.

D. Metric structure in discrete calculus

In the theory of LDG, a metric matrix $M_p$ and its associated inner product are typically endowed for each $p$. To contrast it with the Legendre duality introduced later, we briefly outline it here. For an edge-weighted graph $G_{k \pm}$ and for the case that $k^+ = k^- = k \in \mathbb{R}^N_{>0}$,\textsuperscript{26} As far as we know, we do not have a systematic and widely-appreciated way to define these bases because we have multiple ways to extend the notion of spanning tree of a graph to a hypergraph.\textsuperscript{27} These notations are consistent with those in Sec. II.\textsuperscript{28} If we define 3-cells, then the proper divergence is defined as the differentials $C^2(G) \rightarrow C^3(G)$.\textsuperscript{29} This convention is confusing because, in the theory of differential form, the divergence is identified with $\delta^2 : C^2 \rightarrow C^3$. This is because $C^3$ can be isomorphic to $C^0$ via the Hodge star operator in the three dimensional Euclidean space\textsuperscript{72}. In algebraic graph theory, the trivial metric, i.e., the identity matrix, is implicitly employed when $\text{grad}^*_B$ is identified with $\text{div}_B$\textsuperscript{94}.
\( M_0 = I \) and \( M_1 = \text{diag}[1/k] \) are conventionally employed. With these metric matrices, the graph Laplacian introduced in Eq. 5 can be described as

\[
\mathcal{L}_k = \text{div}_g M^1 \text{grad}_g M_0
\]  

where \( M^p := M_p^{-1} \). By including such metric information, the following pair of metric gradient and divergence is often used in graph theory and network theory: \( \text{grad}_M := \sqrt{M^T B^T} \) and \( \text{div}_M := B \sqrt{M^T} \) where \( \sqrt{M^T} := \text{diag}[\sqrt{k}] \). This symmetric graph Laplacian \( \mathcal{L}_k \) induces a linear dynamics on graph via Eq. 6:

\[
\dot{x} = -\mathcal{L}_k x.
\]  

The eigenvalues and eigenvectors of \( \mathcal{L}_k \) enable us to obtain spectral information of the underlying graph\[95\]. Even for nonlinear dynamics on a hypergraph as in Eq. 14, the same symmetric Laplacian can provide some information when \( k^+ = k^- = k \). We can also include other information in the metric such as the degree of vertices\[111\]. Various normalizations of the graph Laplacian can be attributed to the choice of metrics.

However, such a choice of metric matrices ends up only with linear dynamics and is relevant only when the weighting is symmetric: \( k^+ = k^- = k \). In addition, it may not always capture important aspects of the dynamics such as gradient flow properties and information-theoretic properties, because nonlinear terms such as \( \ln p \) appear in information-theoretic quantities. To extend the class of dynamics being covered and to enable the information-geometric characterization of dynamics, we have to generalize the conventional inner product structure by replacing it with the Hessian-information geometric structure induced by convex functions.

**IV. DUALLY FLAT SPACES ON VERTICES AND EDGES AND GENERALIZED FLOW**

In this section, we introduce two pairs of dually flat spaces (Fig. 1): one is associated with the vertex spaces, i.e., the dual spaces of 0-chains and 0-cochains. The other corresponds to the edge spaces, i.e., the dual spaces of 1-chains and 1-cochains. By combining them, the dynamics on graphs and hypergraphs are characterized as a generalized flow.
A. Dually flat spaces on vertices and thermodynamic functions

We work on the density $\mathbf{x}$ and the vertex space for CRN because its reduction to rLDG is straightforward. For a probability vector $\mathbf{p}$, the introduction of dually flat spaces of $\mathbf{p}$ and $\ln \mathbf{p}$ is natural from the information-geometric viewpoint. In CRN, $\mathbf{x}$ is the vector of concentrations of molecular species. As we recently clarified[47, 101], the dually flat spaces, in this case, result from the Legendre duality between extensive and intensive variables in thermodynamics, which is also natural from the physical viewpoint.

**Definition 11** (Primal vertex space (density spaces)). The primal vertex space (also called density space) is the positive orthant $\mathcal{X} := \mathbb{R}^{N_x}_+ \setminus \{0\}$ of the vector space $\mathbb{R}^{N_x}$, together with an isomorphism $\mathbb{R}^{N_x} \simeq C_0(\mathbb{R})$ (Fig. 1, lower left).

**Remark 4.** The density space $\mathcal{X}$ is defined as the positive orthant rather than as $\mathbb{R}^{N_x}_+ \setminus \{0\}$, which excludes the cases where some elements of $\mathbf{x}$ become 0. From the viewpoint of information geometry, this restriction is necessary to consider densities with the same support (all $\mathbf{x}$ in $\mathcal{X}$ should be equivalent in terms of absolute continuity of measures). From the viewpoint of dynamical systems, depending on the specific functional form of the flux $j(\mathbf{x})$, the trajectory $\mathbf{x}(t)$ may not be restricted within $\mathcal{X}$ as $\mathbf{x}(t) \in \mathcal{X}$ for $t \in [0, \infty]$. The property $\mathbf{x}(t)$ in $\mathcal{X}$ for $t \in [0, \infty]$ is known as persistence[30]. Without going into this intricate problem, we simply assume that $\mathbf{x}(t) \in \mathcal{X}$ for $t \in [0, \infty]$. We call $\partial \mathcal{X} := \mathbb{R}^{N_x}_+ \setminus \mathcal{X}$ the boundary of $\mathcal{X}$.

We define the dual vertex space by the Legendre transform via the thermodynamic function:

**Definition 12** (Primal thermodynamic function). A strictly convex differentiable function $\Phi(\mathbf{x}) : \mathcal{X} \to \mathbb{R}$ is called the primal thermodynamic function[31][32] if the following two conditions we introduced.

---

[30] The persistence of a dynamical system is a hard problem, and the persistence for a subclass of CRN was an open problem until very recently[112, 113], which goes by the name of Global Attractor Conjecture since 1974.

[31] In information geometry, the convex function inducing duality is often called a potential function. We avoid using the word “potential” to discriminate it with an element of the dual vertex space, which is called a potential (field) or chemical potential in physics and chemistry. In addition, “thermodynamic” implies the additional two conditions we introduced.

[32] We may consider a convex function $\Phi(\mathbf{x})$, which
conditions are satisfied: (1) the associated Legendre transformation

\[ \partial \Phi : \mathcal{X} \to \mathbb{R}^{N_x} \]

\[ x \mapsto y := \partial_x \Phi(x) = \left( \frac{\partial \Phi(x)}{\partial x_1}, \ldots, \frac{\partial \Phi(x)}{\partial x_{N_x}} \right)^T \]

has the image \( Y := \{ y | y = \partial \Phi(x), x \in \mathcal{X} \} \) being equal to \( \mathbb{R}^{N_x} \), i.e., \( Y = \mathbb{R}^{N_x} \); (2) for any \( x_{in} \in \mathcal{X} \) and any point on the boundary \( x_{bd} \in \mathbb{R}_{\geq 0}^{N_x} \setminus \mathcal{X} \),

\[ \lim_{\lambda \to +0} \frac{d\Phi(x_\lambda)}{d\lambda} = -\infty \]

holds where \( x_\lambda := \lambda x_{bd} + (1 - \lambda) x_{in} \) for \( \lambda \in [0, 1] \).

**Definition 13** (Dual vertex space (potential space) and dual thermodynamic function).

The dual vertex space \( Y = \mathbb{R}^{N_x} \) called potential (field) space is an affine space dual to \( \mathcal{X} \) with the associated vector space \( C^0(\mathbb{H})((\text{Fig. 1, upper left}))^{[33]} \). The dual thermodynamic function \( \Phi^*(y) : Y \to \mathbb{R} \) is the Legendre-Fenchel conjugate of the primal thermodynamic function:

\[ \Phi^* : Y \to \mathbb{R}, \quad y \mapsto \Phi^*(y) := \max_{x' \in \mathcal{X}} [\langle x', y \rangle - \Phi(x')] \]

(24)

where \( \langle \cdot, \cdot \rangle : C_0(\mathbb{H}) \times C^0(\mathbb{H}) \to \mathbb{R} \) is the bilinear pairing under the standard basis. From the properties of the primal function, \( \Phi^*(y) \) is also a strictly convex differentiable function. From \( \Phi^*(y) \), we have the inverse Legendre transformation \( \partial \Phi^* : Y \to \mathcal{X}, \ y \mapsto x = \partial_y \Phi^*(y) \).

The Legendre transformations, \( \partial \Phi \) and \( \partial \Phi^* \), are continuous and establish a bijection between \( \mathcal{X} \) and \( Y \), where \( \partial \Phi^* = \partial \Phi^{-1} \). In the following, we regard a pair \((x, y)\) with the same decoration as a Legendre dual pair satisfying \( y = \partial \Phi(x) \). For a pair, the Legendre-Fenchel-Young identity holds:

\[ \Phi(x) + \Phi^*(y) = \langle x, y \rangle \]

(25)

Different pairs are discriminated with the difference of decorations as \((x', y')\) or \((x_p, y_p)\).

Based on the thermodynamic functions, the Bregman divergences can be defined:

---

[33] Y is associated with the 0-cochain. In the theory of differential forms, a 0-form is often described as a potential field on a manifold. Our choice of the potential space is consistent with this convention.
We here used the Legendre-Fenchel-Young identity and \(G\) when they are twice differentiable and \(y\) because \((x, y)\) abbreviated as Bregman divergences [1, 114]. Furthermore, from the strict convexity of the thermodynamic function, \(D^X_\Phi[x||x']\) is also strictly convex with respect to \(x\) and \(D^X_\Phi[x'||x] = 0\) if and only if \(x = x'\). Bregman divergences are defined for \((y, y')\) and also for \((x, y')\) as

\[
D^X_\Phi[y'\|y] := \Phi^*(y') - \Phi^*(y) - \langle \partial \Phi^*(y), y' - y \rangle,
\]

\[
D^{X,Y}_{\Phi^*,\Phi}[x\|y'] := \Phi(x) + \Phi^*(y') - \langle x, y' \rangle.
\]

Because \((x, y)\) and \((x', y')\) are Legendre pairs, all the three representations are equivalent [34]: \(D^X_\Phi[x\|x'] = D^{X,Y}_{\Phi^*,\Phi}[y'\|y] = D^{X,Y}_{\Phi^*,\Phi}[x\|y']\). \(D^X_\Phi[x\|x'], D^{Y}_{\Phi^*,y}[y\|y], \) and \(D^{X,Y}_{\Phi,\Phi^*}[x\|y']\) are abbreviated as \(D^X[x\|x'], D^Y[y\|y], \) and \(D^{X,Y}[x\|y']\), respectively.

Finally, the Hessian matrices of the primal and dual thermodynamic functions are defined when they are twice differentiable [36]:

**Definition 15** (Hessian matrices). The primal and dual Hessian matrices, \(G_x \in \mathbb{R}^{N_x \times N_x}\) and \(G^*_y \in \mathbb{R}^{N_y \times N_y}\), of thermodynamic functions, \(\Phi(x)\) and \(\Phi^*(y)\), are defined as

\[
(G_x)_{i,j} := \frac{\partial^2 \Phi(x)}{\partial x_i \partial x_j}, \quad (G^*_y)_{i,j} := \frac{\partial^2 \Phi^*(y)}{\partial y_i \partial y_j}.
\]

In addition, they are positive definite [37] and \(G^{-1}_x = G^*_y\) holds for a Legendre dual pair \(x\) and \(y\).

The Hessian matrices induce linear mappings between the tangent spaces \(T_x \mathcal{X}\) and \(T_y \mathcal{Y}\) where \(T_x \mathcal{X}\) and \(T_y \mathcal{Y}\) are isomorphic to the corresponding cotangent spaces \(T^*_y \mathcal{Y}\) and \(T^*_x \mathcal{X}\) and also to copies of \(C_0(\mathbb{H})\) and \(C^0(\mathbb{H})\): \(T_x \mathcal{X} \cong T^*_y \mathcal{Y} \cong C_0(\mathbb{H})\) and \(T_y \mathcal{Y} \cong T^*_x \mathcal{X} \cong C^0(\mathbb{H})\).
The typical example of the duality between $x$ and $y$ in statistics is that between $x = p$ and $y = \ln p$. Other than this typical one, depending on the purpose, we adopt or design different forms of thermodynamic functions ($\Phi(x), \Phi^*(y)$), associated dual variables, and Bregman divergence to endow different properties to inference or estimation methods that we are designing[1]. In the case of CRN, the thermodynamic functions and Legendre duality are associated with the equilibrium thermodynamics[118]. Specifically, as we recently demonstrated[119], $\mathcal{X}$ and $\mathcal{Y}$ are the conjugate spaces of the extensive and intensive thermodynamic variables (density of molecules and their chemical potential), $\Phi(x)$ is the thermodynamic potential function of the system, and the Bregman divergence becomes the difference of the total entropy. These correspondences are derived directly from the axiomatic formulation of thermodynamics[118, 119]. The explicit functional form of $\Phi(x)$ is then determined by the physical details of the thermodynamic system that we work on.

Before closing this subsection, we introduce the notion of separability, which will be linked to the locality of the flux.

**Definition 16** (Separability of a thermodynamic function). A thermodynamic function $\Phi(x)$ is separable if it can be represented as

$$\Phi(x) = \sum_{i=1}^{N_v} c_i \phi(x_i/x_0^i),$$

(30)

where $c_i > 0$ and $x_0^i > 0$ are positive weights and $\phi(x) : \mathbb{R}_{>0} \to \mathbb{R}$ is a scalar primal thermodynamic function without condition (2) in Def. 12[38][39].

If $\Phi(x)$ is separable, then its conjugate $\Phi^*(y)$ is also separable as $\Phi^*(y) = \sum_{i=1}^{N_v} c_i \phi^*(x_i^*/c_i y_i)$ where $\phi^*(y) : \mathbb{R} \to \mathbb{R}$ is the Legendre conjugate of $\phi(x)$[40]. If a thermodynamic function is separable, then the corresponding Bregman divergence is separable. The Hessian matrices become diagonal for a separable thermodynamic function. Most of our results can hold without the separability, but common thermodynamic functions and related quantities are typically separable. For example, the Kullback-Leibler divergence is an example of separable Bregman divergences.

---

[38] Separability should not be confused with the separability of topological space. The separability here is motivated by the separability of the multidimensional convolution operation.

[39] The condition (2) is not necessary because it automatically follows from the strict convexity and the condition (1).

[40] One may further generalize the separability such that $\phi(x)$ depends on $i$ as $\phi_i(x)$. 

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B. Dually flat spaces on edges and dissipation functions

Next, we introduce another dually flat structure onto the edge space of graphs and hypergraphs based on the flux-force relation.

**Definition 17** (Primal and dual edge spaces (flux and force spaces)). The flux and force spaces on the edges, $\mathcal{J}_x = \mathbb{R}^{N_e}$ and $\mathcal{F}_x = \mathbb{R}^{N_e}$, are a pair of the primal and dual vector spaces defined for each $x \in \mathcal{X}$, which are isomorphic to the copies of $C_1(H)$ and $C^1(H)$, respectively. The bilinear pairing under the standard basis $\langle \cdot, \cdot \rangle : C_1(H) \times C^1(H) \to \mathbb{R}$ is inherited to $(\mathcal{J}_x, \mathcal{F}_x)$.

To introduce Legendre duality on $(\mathcal{J}_x, \mathcal{F}_x)$, we use the dissipation functions:

**Definition 18** (Dissipation function). A dissipation function on $\mathcal{F}_x$, $\Psi^*_x : \mathcal{F}_x \to \mathbb{R}, f \mapsto \Psi^*_x(f)$, is a strictly convex and continuously differentiable function with respect to $f$ for all $x \in \mathcal{X}$ that also satisfies the following additional conditions:

1-coercive: $\frac{\Psi^*_x(f)}{||f||} \to \infty$ as $||f|| \to \infty$,

Symmetric: $\Psi^*_x(f) = \Psi^*_x(-f)$

Bounded below by 0: $\Psi^*_x(0) = 0$.

**Proposition 1** (Duality of dissipation functions). *The Legendre-Fenchel conjugate of $\Psi^*_x(f)$, i.e., $\Psi_x(j) := \max_f [\langle j, f \rangle - \Psi^*_x(f)]$, is also the dissipation function on $\mathcal{J}_x$. $\Psi_x(j)$ and $\Psi^*_x(f)$ are called primal and dual dissipation functions.*

*Proof.* For each $x \in \mathcal{X}$, the function $\Psi_x(j)$ is strictly convex, continuously differentiable, 1-coercive, and $\Psi_x(j) < +\infty$ for all $j \in \mathbb{R}^{N_e} = \mathcal{J}_x$ because $\Psi^*_x(f)$ is (Corollary 4.1.4 in [120]). For $j \in \mathcal{J}_x$, the symmetry holds as $\Psi_x(-j) = \max_f [\langle -j, f \rangle - \Psi^*_x(f)] = \max_f [\langle j, -f \rangle - \Psi^*_x(f)] = \max_f [\langle j, f \rangle - \Psi^*_x(-f)] = \max_f [\langle j, f \rangle - \Psi^*_x(f)] = \Psi_x(j)$.

From the convexity and symmetry, the minimum of $\Psi_x(j)$ is attained at $j = 0$ and $\min_j \Psi_x(j) = \Psi_x(0) = \max_f [\langle 0, f \rangle - \Psi^*_x(f)] = -\min_f \Psi^*_x(f) = 0$. □

[41] While we introduced the affine spaces for $\mathcal{X}$ and $\mathcal{Y}$ associated with $C_0(H)$ and $C^0(H)$, we here directly associate $\mathcal{J}_x$ and $\mathcal{F}_x$ with $C_1(H)$ and $C^1(H)$.

[42] The definition of dissipation functions is more strict than those used in the previous works, e.g., [74]. This is because we define generalized projections in this space as in [82].
From these properties, for each \( x \in X \), the one-to-one Legendre duality via Legendre transformations is established for all over \((J_x, F_x)\):

\[
j = \partial_f \Psi_x^*(f), \quad f = \partial_j \Psi_x(j).
\] (34)

In the following, we abbreviate the Legendre transformations as \( \partial_f \Psi_x^*(f) = \partial \Psi_x^*(f) \) and \( \partial_j \Psi_x(j) = \partial \Psi_x(j) \) \([43]\). Similarly to the Legendre dual pair \((x, y)\) in the spaces \( X \) and \( Y \), a pair of flux and force with the same decoration, e.g., \((j, f)_x\) or \((j_0, f_0)_x\), represents a Legendre dual pair linked by Eq. 34 at \( x \). We omit the \( x \)-dependency for simplicity. The Legendre dual pair \((j, f)\) satisfies the Legendre-Fenchel-Young identity for each \( x \in X \):

\[
\Psi_x^*(f) + \Psi_x(j) - \langle j, f \rangle = 0.
\] (35)

Furthermore, the additional conditions of dissipation functions endow the Legendre duality with the properties necessary to work as an extension of a Riemannian metric structure:

**Proposition 2** ([74]). The Legendre transformations satisfy the following properties:

\[
(Pairing of 0 \in J \text{ and } 0 \in F): \quad 0 = \partial \Psi_x^*(0), \quad 0 = \partial \Psi_x(0) \quad (36)
\]

\[
(Symmetry): \quad -f = \partial \Psi_x(-j), \quad -j = \partial \Psi_x^*(-f). \quad (37)
\]

\[
(Nonnegativity of bilinear pairing): \quad \langle j, f \rangle = \Psi_x^*(f) + \Psi_x(j) \geq 0. \quad (38)
\]

The first property means that zero force \( f = 0 \) and zero flux \( j = 0 \) are always Legendre dual regardless of \( x \), and the second one indicates that if \((j, f)\) is a Legendre dual pair, then \((-j, -f)\) is one as well\([44]\). The third property, as well as the nonnegativity of the dissipation functions, enable them to work as extensions of the norm\([45]\).

With the dissipation functions, \( \Psi_x(j) \) and \( \Psi_x^*(f) \), we now have the second dually flat structure on the edge spaces \((J_x, F_x)\). In these dually flat spaces, we define the Bregman divergence and Hessian matrices:

\[\text{[43] We do not use differentiation of } \Psi_x^*(f) \text{ and } \Psi_x(j) \text{ with respect to other variables.}\]

\[\text{[44] From the physical point of view, these conditions are consistent with the thermodynamic requirement that, if the force is zero, the corresponding flux becomes zero, and vice versa and that a sign-reversed force induced the sign-reversed flux.}\]

\[\text{[45] In the context of thermodynamics, the nonnegativity of } \langle j, f \rangle \text{ is linked to the nonnegativity of the entropy production rate and thus the 2nd law of thermodynamics.}\]
Definition 19 (Bregman divergence and Hessian matrices on the edge spaces). For each \( x \in X \), the Bregman divergence between \( j \in J_x \) and \( f' \in F_x \) is defined as
\[
\mathcal{D}_{x}^{J,F}[j; f'] := \Psi_{x}(j) + \Psi_{x}^{*}(f') - \langle j, f' \rangle.
\]
\( \mathcal{D}_{x}^{J}[j; j'] \) and \( \mathcal{D}_{x}^{F}[f; f'] \) are also defined analogously to the Bregman divergence on the vertex space \((X, Y)\). For a Legendre conjugate pair of twice differentiable dissipation functions, the Hessian matrices, \( G_{x,j} \) and \( G_{x,f}^{*} \), are defined as
\[
(G_{x,j})_{e,e'} := \frac{\partial^{2} \Psi_{x}^{*}(j)}{\partial j_{e} \partial j_{e'}}, \quad (G_{x,f}^{*})_{e,e'} := \frac{\partial^{2} \Psi_{x}^{*}(f)}{\partial f_{e} \partial f_{e'}}.
\]
These matrices are positive-definite.

The Legendre dual structure via the dissipation functions provides an extension of a Riemannian metric structure in the following sense. If the dissipation function is a quadratic function, i.e., a positive definite quadratic form as
\[
\Psi_{x}^{q,*}(f) := \frac{1}{2} \langle f, M_{x} f \rangle,
\]
where \( M_{x} \) is a positive definite \( N^{e} \times N^{e} \) matrix, the Legendre transformation is reduced to the linear mapping \( \partial \Psi_{x}^{q,*}(f) = M_{x} f \). Then, the bilinear paring, \( \langle j, f' \rangle = \langle j, M_{x} j' \rangle = \langle M_{x} f, f' \rangle \), becomes the inner product under the metric matrix \( M_{x} \). The dissipation functions are associated with the induced norms: \( \Psi_{x}^{*}(f) = \frac{1}{2} \| f \|_{M_{x}^{*}}^{2} \), \( \Psi_{x}(j) = \frac{1}{2} \| j \|_{M_{x}}^{2} \).

The Bregman divergence is reduced to the norm-induced squared distance:
\[
\mathcal{D}_{x}^{J,F}[j; f'] = \frac{1}{2} \| j - j' \|_{M_{x}}^{2} = \frac{1}{2} \| f - f' \|_{M_{x}^{*}}^{2}.
\]

Finally, we also introduce the notion of separability to the dissipation functions:

Definition 20 (Separability and locality of dissipation functions). A dissipation function \( \Psi_{x}^{*}(f) \) is separable if it can be represented as
\[
\Psi_{x}^{*}(f) = \sum_{e=1}^{N_{e}} \omega_{e}(x) \psi^{*}(f_{e}/f_{e}^{0}(x)),
\]
where \( \omega_{e}(x) > 0 \) and \( f_{e}^{0}(x) > 0 \) for \( x \in X \) are positive weights and \( \psi^{*}(f) : \mathbb{R} \rightarrow \mathbb{R} \) is a scalar dissipation function, i.e., a strictly convex differentiable scalar function satisfying Eq. 32.

[46] This correspondence illustrates that the dependency of \( \Psi_{x}^{q,*}(f) \) on \( x \) is a formal generalization of the Riemannian metric.
Eq. 33, and Eq. 31. If \( \omega(x) \) and \( f_o(x) \) are additionally local, then the dissipation function is separable and local. If \( \Psi_x^*(f) \) is separable, then its dual \( \Psi_x(j) \) is also separable. The same is true for the locality.

**Remark 5 (Young functions and N functions).** The scalar dissipation function is a N function, which appears in the theory of Orlicz spaces. A function \( \tilde{\psi}(j) : [0, \infty) \to [0, \infty] \) represented as \( \tilde{\psi}(j) = \int_0^j \varsigma(j')dj' \) is called Young function where \( \varsigma(j) : [0, \infty) \to [0, \infty] \) is a non-decreasing function satisfying \( \varsigma(0) = 0 \) and being left-continuous on \( (0, \infty) \). If \( \varsigma(j) \) additionally satisfies \( 0 < \varsigma(j) < +\infty (0 < j < \infty) \), \( \lim_{j \to +0} \varsigma(j) = 0 \), and \( \lim_{j \to \infty} \varsigma(j) = +\infty \), then \( \tilde{\psi}(j) \) is called an N-function. If we define a function \( \psi(j) \) with a N-function \( \tilde{\psi}(j) \) as \( \psi(j) = \tilde{\psi}(|j|) \), this becomes a scalar dissipation function[121]. A separable dissipation function (Eq. 42) is often called a weighted N-function[122, 123]. The dissipation function and induced Legendre duality are, therefore, tightly related to Birnbaum-Orlicz spaces, which are an extension of \( L^p \) spaces.

### C. Generalized flow on graphs and hypergraphs and its steady state

Because of the one-to-one Legendre duality between \((j, f)_x\), the continuity equation (Eq. 10) can be represented as a generalized flow driven by the force \( f(x) \) conjugate to \( j(x) \)[76]:

**Definition 21 (Generalized flow).** A curve \( x(t) \) is a generalized flow on \( H \) driven by force \( f(x) \) under the dissipation function \( \Psi_x^* \) if it can be represented as

\[
\dot{x} = -\text{div}_x j(x) = -\text{div}_x \partial \Psi_x^*[f(x)].
\]

This representation is not dependent on the specific functional form of \( f(x) \) and \( \Psi_x^*(f) \) and also on the definition of \( \text{div}_x \) as long as the generated \( j(x) \) is consistent with \( H[47][48] \). Thus, we can potentially apply this framework to various systems by choosing these functions appropriately depending on the system or the problem we work on.

The generalized flow naturally encompasses three types of steady states:

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[47] The consistency is required because of our choice [48] The consistency with \( H \) is assumed to hold. We of \( \mathbb{R}^{N_x}_{\geq 0} \) as the state space. discuss this matter in Discussion.
Definition 22 (Steady state, complex-balanced state, and detailed-balanced state). We define the manifolds of steady state $\mathcal{M}^{\text{ST}}$, complex-balanced (CB) state $\mathcal{M}^{\text{CB}}$, and detailed-balanced (DB) state $\mathcal{M}^{\text{DB}}$, respectively, as follows:

\[ \mathcal{M}^{\text{ST}} := \{ x \in \mathcal{X} | S_j(x) = 0 \} \]
\[ \mathcal{M}^{\text{CB}} := \{ x \in \mathcal{X} | \mathbb{B}j(x) = 0 \} \]
\[ \mathcal{M}^{\text{DB}} := \{ x \in \mathcal{X} | j(x) = 0 \} = \{ x \in \mathcal{X} | f(x) = 0 \} \]

where we used $j(x) = 0$ iff $f(x) = 0$ from the properties of the dissipation functions. The relations $j(x) = 0$ and $\mathbb{B}j(x) = 0$ are called the detail-balanced condition and the complex-balanced condition, respectively. From the decomposition $\mathcal{S} = \mathbb{L} \mathbb{B}$, the inclusion relation holds: $\mathcal{M}^{\text{DB}} \subseteq \mathcal{M}^{\text{CB}} \subseteq \mathcal{M}^{\text{ST}}$. It should be noted that, depending on the details of $j(x)$, these manifolds can be empty.

A steady state is a state at which $\dot{x} = 0$ holds. The DB condition $j(x) = 0$ means that all the fluxes are zero at $x$. In other words, all the forward and reverse fluxes are balanced at $x$, i.e., $j^+(x) = j^-(x)$. The CB condition is equivalent to the balance of all influx and outflux at each hypervertex of $\mathbb{H}$. As we will see later, DB states are tightly linked to the equilibrium state, the steady state of equilibrium flow. The CB state is relevant as an extension of the equilibrium state to nonequilibrium flows.

D. Generalized gradient flow and De Giorgi’s formulation

When $f(x)$ can be represented as a gradient, i.e., $f(x) = \text{grad}_x \partial F(x)$ of a function $F(x) \in \mathbb{R}$ on the density space, Eq. 43 is reduced to the generalized gradient flow of $F(x)$.

Definition 23 (Generalized gradient flow). $x(t)$ is a generalized gradient flow when it is a generalized flow driven by a gradient force of $F(x)$, i.e., $f(x) = \text{grad}_x \partial F(x)$ and

\[ \dot{x} = -\text{div}_x j(x) = -\text{div}_x \partial \Psi_x^*[\text{grad}_x \partial F(x)]. \]

(47)

The following proposition ensures that the generalized gradient flow behaves like the conventional gradient flow:

Proposition 3 ($F(x)$ is non-increasing along the trajectory of generalized gradient flow). For a trajectory $\{x_t\}_{t \in [0,T]}$ of the generalized gradient flow of $F(x)$, $F(x_t)$ is always
decreasing except at the DB states $\mathcal{M}^{DB}$. In addition, all the steady states of the generalized gradient flow are the DB states, i.e., $\mathcal{M}^{ST} = \mathcal{M}^{DB}$.[49]

Proof. $\mathcal{F}(x_t)$ is non-increasing over time as follows:

$$\dot{\mathcal{F}}(x_t) = \langle \dot{x}, \partial_x \mathcal{F}(x) \rangle = -\langle \text{div}_x \Psi_x^*[f(x)], \partial_x \mathcal{F}(x) \rangle = -\langle \partial_x \Psi_x^*[f(x)], \text{grad}_x \partial_x \mathcal{F}(x) \rangle$$

$$= -\langle j(x), f(x) \rangle = \Psi_x[j(x)] + \Psi_x^*[f(x)] \leq 0,$$

(48)

where Eq. 38 is used. The equality holds iff $f(x) = \text{grad}_x \mathcal{F}(x) = 0$ because $\Psi_x^*[f(x)] = \Psi_x[j(x)] = 0$ iff $f(x) = j(x) = 0$. Thus, $\dot{\mathcal{F}}(x_t) = 0$ iff $x_t \in \mathcal{M}^{DB}$. Because $\dot{x}_t = 0 \Rightarrow \dot{\mathcal{F}}(x_t) = 0$, $\mathcal{M}^{ST} = \mathcal{M}^{DB}$.

It should be noted that, even if $\mathcal{F}(x)$ has a single minimum, the steady state $x_{st} := \lim_{t \to \infty} x(t)$ may not be the minimum, because $\dot{\mathcal{F}}(x_t) = 0$ holds for any $x \in \mathcal{M}^{DB}$.[50]

The generalized gradient flow of this form (Eq. 48) was devised in the process to extend the conventional gradient flow to metric spaces[124, 125][51]. Furthermore, dissipation functions have been recognized since the seminal work of Onsager[126–128]. However, only quadratic dissipation functions have been investigated until very recently[74–81]. This may be partly because we lack an adequate geometric language to handle the non-quadratic cases, i.e., information geometry[52]. Actually, if the dissipation function is quadratic $\Psi^q_x[f]$ as in Eq. 41, then the generalized flow (Eq. 43) formally reduces to the flow on a Riemannian manifold with the metric $S M_x^* S^T$.

The non-negativity of $\dot{\mathcal{F}}(x_t)$ is essentially attributed to the fact that $\dot{\mathcal{F}}(x_t) = -\langle j(x), f(x) \rangle$ holds in Eq. 48 for the generalized gradient flow. The converse also holds.

Proposition 4 (De Giorgi’s formulation of generalized gradient flow[74, 78]). Let $x_t$ be a generalized flow induced by a force $f(x)$. $x_t$ is the generalized gradient flow of $\mathcal{F}(x)$ iff

$$\dot{\mathcal{F}}(x_t) = -\langle j(x), f(x) \rangle = - (\Psi_x[j(x)] + \Psi_x^*[f(x)]).$$

(49)

Another reason is that the generalized gradient flow was devised to investigate infinite-dimensional partial differential equation, in which the formally obtained results via the gradient flow structure should be rigorously proven via a different approach.

[49] $\mathcal{M}^{ST} = \mathcal{M}^{DB} = \emptyset$ can hold, e.g., when $\mathcal{F}(x)$ is a strictly monotonous function.

[50] In addition, there exists the possibility that $x(t)$ converges to the boundary of $\mathcal{X}$.

[51] The metric here means a general metric, which is not restricted to one associated with the inner product.
holds. The integral form of Eq. 49
\[ F(x_0) - F(x_t) = \int_0^t \left[ \Psi_{x_{t'}}(f(x_{t'})) + \Psi_{x_{t'}}(j(x_{t'})) \right] \, dt', \] (50)
is called De Giorgi’s \((\Psi, \Psi^*)\)-formulation of generalized gradient flow.

Proof. For a generalized flow \(x_t\) driven by force \(f(x)\) as in Eq. 43 and for any \(F(x)\), the following inequality holds:
\[ \dot{F}(x_t) = \left\langle \dot{x}, \frac{\partial F(x_t)}{\partial x} \right\rangle = \left\langle -j(x_t), \text{grad}_S \frac{\partial F(x_t)}{\partial x} \right\rangle \]
\[ = - \left[ \Psi_{x_t}(j(x_t)) + \Psi^*_{x_t}(f'(x_t)) \right] + D_{x_t}^{\mathcal{J}, F}[j(x_t); f'(x_t)] \] (52)
\[ \geq - \left[ \Psi_{x_t}(j(x_t)) + \Psi^*_{x_t}(f'(x_t)) \right], \] (53)
where we define \(f'(x) := \text{grad}_S \partial F(x)\). The last inequality becomes an equality if and only if \(f'(x_t)\) is the Legendre dual of \(j(x_t)\)[53], i.e.,
\[ D_{x_t}^{\mathcal{J}, F}[j(x_t); f'(x_t)] = 0 \iff j(x_t) = \partial \Psi^*_{x_t}[f'(x_t)] \] (54)
Thus, Eq. 49 holds only when \(x_t\) is the generalized gradient flow of \(F(x)\). \qed

De Giorgi’s formulation is a well-established approach for defining gradient flow in metric spaces[124].

E. Equilibrium and nonequilibrium flow

In this work, we mainly focus on the case that \(F(x) = D_{\Phi}^X[x\|\bar{x}]\) where \(D_{\Phi}^X\) is the Bregman divergence associated with a thermodynamic function \(\Phi\).

Definition 24 (Equilibrium gradient force and equilibrium flow). The force generated by the gradient of Bregman divergence associated with a thermodynamic function \(\Phi\) is called the equilibrium gradient force, and the following equation is denoted as the thermodynamic gradient equation:
\[ f(x) = \text{grad}_S \partial D_{\Phi}^X[x\|\bar{x}], \] (55)

[53] The inequality and the equality condition are usually derived by using Cauchy-Schwarz inequality[129]. From the information-geometric framework, they are trivially attributed to the non-negativity of Bregman divergence.
where $\bar{x} \in \mathcal{X}$ is a parameter. A generalized flow $x(t)$ is an equilibrium flow if it is driven by the thermodynamic gradient force:

$$\dot{x} = -\text{div}_S \partial \Psi_x^* \left[ \text{grad}_S \partial \mathcal{D}_\Phi \left[ x \parallel \bar{x} \right] \right].$$

Using the relation $\partial \mathcal{D}_\Phi^x \left[ x \parallel \bar{x} \right] = \partial \Phi(x) - \bar{y}$ where $\bar{y} = \partial \Phi(\bar{x})$, Eq. 56 can be rewritten as

$$\dot{x} = -\text{div}_S \left[ \partial \Psi_x^* \left[ \text{grad}_S \left\{ \partial \Phi(x) - \bar{y} \right\} \right] \right],$$

which explicitly shows the contribution of both the thermodynamic function and the dissipation function to the dynamics (Fig. 3 (a)).

Various properties of the equilibrium flow (Eq. 56) can be obtained from the dually flat structures as we will see in the following sections. In addition, the equilibrium flow captures the properties that the dynamics of thermodynamic equilibrium systems should hold. In this sense, the equilibrium flow is the mathematical representation of the dynamics of equilibrium systems.

Beyond the gradient equilibrium flow, we also consider the non-gradient nonequilibrium flow of the following type:

**Definition 25** (Nonequilibrium force and nonequilibrium flow). The force generated by the constant shift of the thermodynamic gradient force

$$f(x) = \text{grad}_S \partial \mathcal{D}_\Phi^x \left[ x \parallel \bar{x} \right] + f_{NE},$$

FIG. 3. Schematic representation of the equilibrium (a) and nonequilibrium flow (b).
is called nonequilibrium force where \( f_{NE} \not\in \text{Im}[S^T] \)[54]. If the shift parameter \( f_{NE} \) satisfies \( f_{NE} \in \text{Im}[S^T] \), then the nonequilibrium force is reduced to the equilibrium force \( f_{NE} = 0 \) by appropriately changing \( \tilde{x} \). The nonequilibrium flow is the flow induced by the nonequilibrium force (Fig. 3 (b)):

\[
\dot{x} = -\text{div}_S \partial \Psi_x^* \left( \left[ \text{grad}_S \partial_x D^X_\Phi[x||\tilde{x}] \right] + f_{NE} \right).
\] (59)

In the next section, we show that this equation can cover a sufficiently wide class of models, e.g., all types of rLDG and CRN with extended LMA kinetics. Equation 59 can also be associated with nonequilibrium dynamics with a constant environmental force. The techniques in information geometry, Hessian geometry, and convex analysis enable us to investigate such non-gradient dynamics.

**Remark 6 (Variational modeling[130])**. We introduced and characterized dynamics based on the thermodynamic functions and dissipation functions. While we employed a restricted definition to link dynamics to information geometry, we may further generalize this approach by appropriately choosing the state space, \( f(x), \Psi_x^*(f) \), and \( \text{div}_S \). For example, we may consider a \( x \)-dependent and noninteger-valued stoichiometric matrix \( S(x) \). The equilibrium flow may not be restricted to \( \mathcal{F}(x) = D^X_\Phi[x||\tilde{x}] \), and the nonequilibrium flow may be defined for \( x \)-dependent \( f_{NE}(x) \). This type of approach for modeling dissipative dynamics has been known as variational modeling.

Before closing this section, we mention that the existence of DB states, i.e., \( \mathcal{M}^{\text{DB}} \neq \emptyset \) is necessary and sufficient for a nonequilibrium flow to be the equilibrium flow.

**Proposition 5** (Detailed balance condition and equilibrium flow). Consider a nonequilibrium flow given by Eq. 59. If \( \mathcal{M}^{\text{DB}} \neq \emptyset \), then the flow is equilibrium, i.e., \( f_{NE} \in \text{Im}S^T \).

**Proof.** \( \mathcal{M}^{\text{DB}} \neq \emptyset \) means that there exists \( x_{DB} \) satisfying \( j(x_{DB}) = 0 \). From \( j(x_{DB}) = 0 \Leftrightarrow f(x_{DB}) = 0 \). If \( f_{NE} \not\in \text{Im}[S^T] \), \( f_{NE} \neq 0 \) and thus \( f(x) \neq 0 \) for all \( x \in \mathcal{X} \). Thus, \( f_{NE} \in \text{Im}[S^T] \) if \( \mathcal{M}^{\text{DB}} \neq \emptyset \). \( \square \)

The necessity follows basically from Prop. 3, but we have to show \( \mathcal{M}^{\text{ST}} \neq \emptyset \). This will be shown in the following section (Lemma 1).

[54] In physics, such \( f_{NE} \) can be identified with a nonequilibrium force applied externally to the system.
V. EXPLICIT FORM OF THERMODYNAMIC AND DISSIPATION FUNCTIONS

Before investigating the dynamics of the equilibrium (Eq. 56) and nonequilibrium (Eq. 59) flow, we show how the flow can be associated with the dynamics on graphs and hypergraphs via specific forms of the thermodynamic and dissipation functions. The forms of functions depend on the functional form of the flux that we assume: Eq. 3 for rLDG, Eq. 12 for CRN with LMA kinetics, and Eq. 16 for FPE. It should be noted that the choice of the thermodynamic function and the dissipation function is not unique for a given dynamics in general. Depending on the purpose, we should choose or find an appropriate set of functions.

A. Thermodynamic and dissipation functions for symmetric rLDG

The symmetric rLDG defined by Eq. 20 is treated as an illustrative example. From the form of the graph Laplacian (Eq. 19)\(^{[55]}\), it is easy to see that Eq. 20 coincides with Eq. 56 if

\[
\Phi(x) = \frac{1}{2} \langle x, M_0 x \rangle, \quad \Psi_x^*(\mathbf{f}) = \frac{1}{2} \langle \mathbf{f}, M^1 \mathbf{f} \rangle, \quad (60)
\]

where \( \mathcal{Y} = \mathcal{X} \), \( M_0 = I \), \( M^1 = \text{diag}[k] \), and \( \bar{x} = 0^{[56]} \). Because both \( M_0 \) and \( M^1 \) are diagonal, these thermodynamic and dissipation functions are separable.

\(^{[55]}\) It should be noted that this representation holds only when \( k^+ = k^- \) holds.

\(^{[56]}\) While \( \mathcal{Y} \neq \mathbb{R}^{N_x} \), no problem arises because \( M_0 \) is the trivial identity matrix in this case. Also, this
B. Explicit form of thermodynamic functions for rLDG and CRN

For rLDG (Eq. 3) and CRN with LMA kinetics (Eq. 12), the following dual thermodynamic functions are particularly relevant\[^{57}\]:

\[
\Phi(x) := \ln x - \ln x^o - 1, \quad \Phi^*(y) := (x^o)^T e^y = \sum x^o_i e^{y_i},
\]

which induce the following Legendre transformation:

\[
y = \partial \Phi(x) = \ln x - \ln x^o, \quad x = \partial \Phi^*(y) = x^o \circ e^y.
\]

Here, \( Y = \mathbb{R}^{N_x} \), and \( x^o \in X \) is a parameter determining the point in \( X \) that is associated with the origin of \( Y \) via the Legendre transformation. For these thermodynamic functions, the Bregman divergence is reduced to the generalized Kullback-Leibler divergence.

\[
\mathcal{D}^X[p||p'] = \left( \ln \frac{x}{x'} \right)^T x - 1^T (x - x').
\]

These thermodynamic functions and the Bregman divergence are separable.

If we choose \( x^o = 1 \), then the conventional dual representation for the distribution \( p \) on a discrete space is recovered:

\[
\Phi(p) = \ln p - 1^T p, \quad \Phi^*(y) = 1^T e^y, \quad y = \partial_p \Phi(p) = \ln p, \quad p = \partial_y \Phi^*(y) = e^y,
\]

where we use \( p \) instead of \( x \). In this case, \( Y \) is the space of the logarithm of \( p \). These representations hold even if \( p \) is not a probability density. If \( p \) satisfies \( 1^T p = 1 \), the generalized KL divergence becomes the normal KL divergence \( \mathcal{D}^Y[p||p'] = \left( \ln \frac{p}{p'} \right)^T p \). [58]

\[^{57}\] For CRN, these forms of the thermodynamic functions are derived from the macroscopic thermodynamics of ideal gas or dilute solution with non-reactive solvent[119]. Mathematically, we may employ other functions for the same MJP or CRN with LMA kinetics as we introduce different information geometric structures onto a family of probability depending on the purpose. Such an exploitation is an interesting open problem.

\[^{58}\] As we will see later, the condition \( 1^T p(t) = 1 \) need not be assumed but is automatically satisfied due to the topological constraint of the graph and the initial condition \( 1^T p(0) = 1 \) when we work on rMJP.
C. Explicit form of dissipation functions for rLDG and CRN

To determine the dissipation functions, we need the definition of force, which may depend on the phenomena and purpose\[59\]. In physics, the flux-force relations, which are also called constitutive equations\[131\], are central because they determine what kind of change is induced by an incurred force\[60\]. For rMJP and CRNs, the flux and force are conventionally defined using the one-way fluxes, $j^+(x)$ and $j^-(x)$ as

$$j = j^+ - j^-,$$

$$f = \ln j^+ - \ln j^-,$$  \hspace{1cm} (65)

where the dependency of $j^- (x)$ on $x$ is abbreviated for notational simplicity. In physics, assuming this form of force-flux relation goes by the name of the local detailed balance (LDB) assumption\[61\], or the generalized detailed balance assumption\[62\]. By defining the frenetic activity \[134\]:

$$\omega := 2\sqrt{j^+ \circ j^-} \in \mathbb{R}_{\geq 0}^N,$$  \hspace{1cm} (66)

we have a relation $j = \omega \circ \left[ \exp(f/2) - \exp(-f/2) \right]$. For a fixed $\omega$, this relation between the pair $(j, f)$ is a one-to-one Legendre duality induced by the following specific form of dissipation functions:

$$\Psi^*_\omega(f) := 2\omega^T [\cosh(f/2) - 1],$$

$$\Psi_\omega(j) := 2\omega^T \left( \text{diag} \left[ \frac{j}{\omega} \right] \sinh^{-1} \left( \frac{j}{\omega} \right) - \left[ \sqrt{1 + \left( \frac{j}{\omega} \right)^2} - 1 \right] \right),$$  \hspace{1cm} (67)

which lead to the Legendre transformation:

$$j = \partial \Psi^*_\omega(f) = \omega \circ \sinh(f/2),$$

$$f = \partial \Psi_\omega(j) = 2 \sinh^{-1} \left( \frac{j}{\omega} \right).$$  \hspace{1cm} (68)

\[59\] This is parallel to the problem of how to define the dual of $x$. The choice of logarithm is contingent on the domain and knowledge of physics and statistics.

\[60\] Actual forms of the relations depend on the respective phenomena. Some relations were obtained empirically through experiments and others were computed theoretically from microscopic models.

\[61\] LDB is different from the DBC, which was discussed in Def. 22.

\[62\] The validity of LDB was shown for rMJP and CRN with LMA kinetics via large deviation theory for the corresponding microscopic Markovian models or via its consistency with the macroscopic chemical thermodynamics\[132, 133\].
We can easily verify that these functions satisfy the conditions for dissipation functions, i.e., Eq. 32, Eq. 33, and Eq. 31.

For the flux $j_{MA}(x)$ of LMA kinetics (Eq. 12), the force and activity become

$$f_{MA}(x; K) = \ln K + S^T \ln x,$$
$$\omega_{MA}(x; \kappa) = 2 \kappa \circ x \left[ (B^++B^-) \right]^{T/2}.$$  \(69\)

where we introduced a transformation of the kinetic parameters $(k^+, k^-)$ into the force part $K$ and activity part $\kappa$ as $\kappa := \sqrt{k^+ \circ k^-}$ and $K := k^+/k^-$. Because $k^\pm = \kappa \circ K^{\pm1/2}$ holds, $(\kappa, K)$ has the same information as $(k^+, k^-)$. Moreover, we can verify that the force and activity are dependent only on $K$ and $\kappa$, respectively. The dissipation functions of the forms above and their relations to LDG and CRN were derived from the large deviation function of the corresponding microscopic stochastic models for rMJP and CRN [74, 135]. Actually, the Bregman divergence $D^T_x[j; j_{MA}(x)]$ of the dissipation functions is identical to the rate function of the flux for rMJP and CRN. Thus, these dissipation functions are keystones connecting macroscopic and microscopic dynamics.

If there exists $\tilde{y}$ satisfying $-S^T \tilde{y} = \ln K$, i.e., $\ln K \in \text{Im} S^T$, the force in Eq. 69 is represented as

$$f_{MA}(x; K) = \text{grad}_x \left( \ln \frac{x}{\tilde{x}} \right) = \text{grad}_x \partial_x D^X[x\|\tilde{x}] \in \text{Im} S^T,$$  \(70\)

where $\tilde{x}$ is the Legendre conjugate of $\tilde{y}$. Thus, CRN (and rMJP) is an equilibrium flow of the generalized KL divergence $D^X[x\|\tilde{x}]$ when the parameter $K$ satisfies $\ln K \in \text{Im} S^T$. In chemistry, the condition $\ln K \in \text{Im} S^T$ is called Wegscheider’s equilibrium condition [46, 136], and the CRN satisfying this parametric condition is called equilibrium CRN [66]. Even if

\[63\] The dissipation functions in Eq. 67 and the induced Legendre transformation in Eq. 68 are not necessarily restricted to these particular types of force and activity. Actually, the extended LMA kinetics (Eq. 13) can also be represented by replacing $\omega_{MA}(x)$ with $\omega_{eMA}(x) = g(x) \circ \omega_{eMA}(x)$. Thus, Eq. 67 could be applied to a wider class of kinetics than Eq. 12.

\[64\] For CRN, $K$ is referred as the equilibrium constant in chemistry.

\[65\] It should be noted that, while $\tilde{y}$ is not uniquely determined by $K$ in general, it does not cause problem. This is clarified in the following section (Sec. VIII) by introducing appropriate affine subspaces. Historically, the equilibrium chemical systems were characterized by macroscopic thermodynamics. The equilibrium condition was derived as the necessary and sufficient condition that the flux of the
\( \ln K \in \text{Im} S^T \) is not satisfied, we can represent \( \ln K = -S^T \tilde{y} + f_{NE} \) with \( f_{NE} \notin \text{Im} S^T \). The force in Eq. 69 is always represented as

\[
f_{MA}(x; K) = \text{grad}_x \left( \ln \frac{\tilde{x}}{x} \right) + f_{NE} = \left[ \text{grad}_x \left[ \partial_x D^X(x||\tilde{x}) \right] + f_{NE} \right],
\]

which leads to the nonequilibrium flow (Eq. 59). Thus, CRN with LMA kinetics as well as rLDG are generally within the class of Eq. 59.

**Remark 7 (Wegscheider’s equilibrium condition and Detailed balance condition).** While we defined equilibrium flow by the specific functional form of force and obtained Wegscheider’s equilibrium condition as the necessary and sufficient condition to have the equilibrium force under LMA kinetics, the equilibrium dynamics is often defined by the existence of the steady state satisfying the DB condition (Eq. 45) in CRN theory. In addition, the DB condition is also often assumed in statistics when we design or analyze a random walk in parameter spaces, e.g., in the Markov Chain Monte Carlo simulations or in other random-walk-based optimization schemes. These two are equivalent for (extended) LMA kinetics. Actually, \( \mathcal{M}^\text{CB} \neq \emptyset \) means that there exists \( x_{DB} \in \mathcal{X} \) such that \( j_{MA}(x_{DB}) = 0 \Leftrightarrow -S^T \ln x_{DB} = \ln K \). From the Fredholm alternative, we obtain the Wegscheider’s equilibrium condition \( \ln K \in \text{Im} S^T \) for the existence of \( x_{DB} \).

**D. Some remarks on the dissipation functions for CRN and rLDG**

The dissipation functions in Eq. 67 have several notable properties. First, they are separable:

\[
\Psi^*_\omega(x)(f) = \sum_{e=1}^{N_e} \omega_e(x) \psi^*(f_e), \quad \Psi_\omega(x)(j) = \sum_{e=1}^{N_e} \omega_e(x) \psi(j_e/\omega_e(x)),
\]

LMA kinetics (Eq. 12) should satisfy to have consistent properties with the thermodynamic equilibrium systems. It was found only recently that the equilibrium properties are mathematically attributed to the generalized gradient flow structure. The DB condition is conventionally adopted because, for example, it makes it easy to obtain an MCMC with a desirable stationary distribution. This nice property comes from the gradient-flow property of the equilibrium flow.
where

\[ \psi^*(f) := 2 \left[ \cosh(f/2) - 1 \right] \in [0, \infty), \quad (73) \]
\[ \psi(j) := 2 \left( j \sinh^{-1}(j) - \sqrt{1 + j^2} - 1 \right) \in [0, \infty). \quad (74) \]

and \( \omega(x) \) is local:
\[ \omega_e(x) = 2 \kappa_e \prod_{i=1}^{N_k} x_i^{(\gamma_i^+ + \gamma_i^-)/2}. \]

The thermodynamic functions in Eq. 61 are also separable. The locality and separability of dissipation functions are important requisites for the cochain complexes on graphs and hypergraphs to function as the discrete versions of differential forms\(^{[68]}\).

Second, the scalar function \( \psi^*(f) \) is the N-function. The N-function of the \((\cosh(f) - 1)\)-type and the associated Orlicz space have been employed for establishing the infinite-dimensional information geometry by Pistone\(^{[71, 137, 138]}\). In functional analysis, Orlicz spaces are a generalization of \(L^p\) spaces, which arise naturally when we work on \(L \log L\) spaces for the divergences and large deviation functions. Hence, the dissipation functions in Eq. 67 are tightly related to such topics.

Finally, the dissipation functions in Eq. 67 are not the unique choice to reproduce the force-flux relation in Eq. 65. The quadratic dissipation functions \( \Psi_{x^*}^q(f) := \frac{1}{2} \langle f, M_x^* f \rangle \) in Eq. 41 with the following diagonal metric tensor can reproduce the relation in Eq. 65:
\[ M_x^* = \text{diag} \left[ \frac{j_e^+(x) - j_e^-(x)}{\ln j_e^+(x) - \ln j_e^-(x)} \right] = \text{diag} \left[ \left( \frac{j_e^+(x) - j_e^-(x)}{\ln j_e^+(x) - \ln j_e^-(x)} \right)_{e^*} \right]. \quad (75) \]

This type of quadratic dissipation function has also been proposed even earlier than the non-quadratic ones\(^{[139–141]}\) and been investigated\(^{[142–144]}\). Its advantage is that the induced geometry is Riemannian, and thus the Hessian information geometric argument is not necessarily required. In addition, this Riemannian geometric structure is related to the formal Riemannian geometric structure of FPE and other diffusion processes on continuous manifolds induced via the \(L^2\)-Wasserstein geometry\(^ { [64, 65]}\) (Fig. 4). Thus, this quadratic dissipation function provides a consistent extension of these results for FPE and diffusion processes to graphs and hypergraphs. Nevertheless, the Hessian information geometric structure functions. In addition, equilibrium thermodynamics does not preclude thermodynamic functions from being nonseparable.
ture with the non-quadratic dissipation functions that we introduce is also another sound generalization of the formal Riemannian geometry of FPE, as we see in the next subsection.

As long as we focus only on the trajectory of the generalized flow (Eq. 43), the difference does not matter because both induce the same dynamics. However, the Bregman divergence of the quadratic dissipation functions is not related to the rate function of the microscopic stochastic models, while that of nonquadratic ones in Eq. 67 is[135]. Thus, if we consider projections of fluxes and forces in the edge spaces, different choices of dissipation functions lead to different projections.

![Diagram showing the relationship between Wasserstein geometry, Riemannian geometry, and information geometry.](image)

**FIG. 4.** A relationship between Wasserstein geometry and information geometry. The formal Riemannian geometric structure appears at their intersection. It should be noted that, while the regions of $L^p$-Wasserstein distance for $p \neq 2$ and nonquadratic dissipation function are not overlapping in this figure, this does not mean that they are unrelated. There may be undiscovered relations between these two regions.

### E. Explicit forms of thermodynamic and dissipation functions for FPE

For FPE, the dual representation of the density $p(r)$ and its logarithm $y(r) = \ln p(r)$ is also relevant. This duality is induced formally by the following thermodynamic functions\[69\]:

\[
\Phi[p] = \int [\ln p(r) - 1] p(r) dr, \quad \Phi^*[y] = \int e^y(r) dr, \tag{76}
\]

the Legendre transformation of which is

\[
y(r) = \frac{\delta \Phi[p]}{\delta p} = \ln p(r), \quad p(r) = \frac{\delta \Phi^*[y]}{\delta y} = e^y(r). \tag{77}
\]

\[69\] The base measure is omitted because this is just a formal one.
The Bregman divergence becomes the KL divergence $D_X[p||p'] = \int dr p(r) \ln \frac{p(r)}{p'(r)}$. In physics, the flux and force for FPE are defined conventionally as

$$j_{FP}[p(r)] = D_0 p(r) \left\{ F(r)/D_0 - \nabla \ln p(r) \right\},$$

$$f_{FP}[p(r)] = D_0^{-1} F(r) - \nabla \ln p(r).$$

(78)

(79)

The dissipation functions associated with the force-flux relation above are

$$\Psi_{FP}^{*,\omega}[f] = \frac{1}{2} \int f(p(r))^T M_{p(r)}^* f(p(r)) dr,$$

$$\Psi_{FP}^{*,\omega}[j] = \frac{1}{2} \int j(p(r))^T M_{p(r)} j(p(r)) dr,$$

(80)

where $M_{p(r)}^* := D_0 \text{diag}[\omega[p(r)]]$, $M_{p(r)} := (M_{p(r)}^*)^{-1}$, and $\omega_i[p(r)] = p(r)$. Thus, the dissipation functions are formally quadratic and positive definite. If $F(r)$ is a gradient of $U(r)$ as $F(r) = D_0 \nabla U(r)$, $f_{FP}[p(r)] = -\nabla \ln \tilde{p}(r)$ holds where $\tilde{p}(r) := \exp[U(r)]$. Then, the dissipation functions, the bilinear pairing $\langle j_{FP}, f_{FP} \rangle$, the EPR $\dot{\Sigma}_{FP}$ in Eq. ??, and the pEPR $\dot{\Sigma}_{FP}^p$ in Eq. ?? formally consolidate into the same quantity:

$$2\Psi_{FP}^{*,\omega}[f_{FP}] = 2\Psi_{FP}^{*,\omega}[j_{FP}] = \langle j_{FP}, f_{FP} \rangle = \dot{\Sigma}_{FP} = \dot{\Sigma}_{FP}^p = D_0 \int p(r) \left( \nabla_r \ln \tilde{p}(r) \right)^2 dr.$$

(81)

The last quantity without $D_0$ is known as relative Fisher information[65, 145] and Hyvärinen divergence[122, 146] between $p$ and $\tilde{p}$. For $U(f) = 0$, it reduces to the Fisher information number $I_F[p]$ in Eq. 1. This consolidation is a source of confusion, as the same quantity for FPE or linear diffusion processes has different names in different contexts and in different disciplines. However, they actually have different definitions, roles, and meanings, which are explicit in the information-geometric formulation.

VI. ORTHOGONAL SUBSPACES, DUAL FOLIATION, AND PYTHAGOREAN RELATION

To investigate the behaviors and properties of the equilibrium (Eq. 56) and nonequilibrium (Eq. 59) flow, especially its topological and algebraic constraint from the graph or hypergraph structure, information geometry and Hessian geometry provide technically the ideal tools. In particular, the four subspaces associated with the cycle and cocycle subspaces of the chain and cochain complexes (Fig. 5) form dual foliations via the Legendre transformation, whose geometric properties are captured by Hessian geometry[1, 147]. It should be noted that the results of this section do not assume the specific forms of the thermodynamic and dissipation functions introduced in Sec. V.
A. Four affine subspaces

Two families of orthogonal affine subspaces are naturally introduced on $X$ and $Y$, respectively, from the topological structure of graph and hypergraph, i.e., $B$ and $S$.

**Definition 26** (Stoichiometric subspaces in $X$). The stoichiometric subspaces are defined as

$$P^{sc}(x_0)^{[70]} := \{ x \in X | x - x_0 \in \text{Im}S \}, \quad x_0 \in X$$  \hspace{1cm} (82)

where $x_0$ is a parameter to specify the position of the subspace (Fig. 5, lower left)$^{[71]}$

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$^{[70]}$ In CRN theory, a stoichiometric subspace is called stoichiometric compatibility class$^{[8]}$.

$^{[71]}$ Because $P^{sc}(x_0)$ is restricted within the positive orthant $X$, $P^{sc}(x_0)$ is a polyhedron. If bounded, it is called a polytope in discrete geometry and also in combinatorial optimization$^{[148]}$. However, we abuse the word (affine) subspace for $P^{sc}(x_0)$, and use polyhedron or polytope when we care about the boundary.
Definition 27 (Equilibrium subspaces in $Y$). The equilibrium subspaces (Fig. 5, upper left) are defined as

$$\mathcal{P}^{eq}(\tilde{y}) := \{ y \in Y | y - \tilde{y} \in \text{Ker} S^T \}, \quad \tilde{y} \in Y.$$  

$\mathcal{P}^{sc}(x_0)$ and $\mathcal{P}^{eq}(\tilde{y})$ are orthogonal to each other: $\langle x - x_0, y' - \tilde{y} \rangle = 0$ for $x \in \mathcal{P}^{sc}(x_0)$ and $y' \in \mathcal{P}^{eq}(\tilde{y})$. Because $S$ and $S^T$ are the discrete differentials, $\delta_1$ and $\delta^0$, $\mathcal{P}^{sc}(x_0)$ and $\mathcal{P}^{eq}(\tilde{y})$ are associated with the 0-cycle and 0-cocycle spaces, respectively.$^{[72]}$

Two other families of orthogonal subspaces are introduced on $J_x$ and $F_x$.

Definition 28 (Iso-velocity subspaces in $J_x$). The iso-velocity subspaces (Fig. 5, lower right) are defined as

$$\mathcal{P}^{vl}(\hat{j}) = \{ j \in J_x | j - \hat{j} \in \text{Ker} S \}, \quad \hat{j} \in J_x.$$  

Definition 29 (Iso-force subspaces in $F_x$). The iso-external-force subspaces, iso-force subspaces in short, (Fig. 5, upper right) are defined as

$$\mathcal{P}^{fr}(f') := \{ f \in F_x | f - f' \in \text{Im} S^T \}, \quad f' \in F_x.$$  

Again, from the correspondence of $\delta_1 = S$ and $\delta^0 = S^T$, $\mathcal{P}^{vl}(\hat{j})$ and $\mathcal{P}^{fr}(f')$ are associated with the 1-cycle and 1-cocycle spaces, respectively.$^{[73]}$. We specifically call $\mathcal{P}^{vl}(0)$ and $\mathcal{P}^{fr}(0)$ zero-velocity subspace and gradient-force (GD-force) subspace, respectively. Their meaning is explained in the next subsection.

B. Meaning of the subspaces

All four subspaces are natural constituents in the theory of algebraic graph theory and homological algebra. Here, we provide their meaning in terms of the dynamics on graphs and hypergraphs.

The stoichiometric and iso-velocity subspaces, $\mathcal{P}^{sc}(x_0)$ and $\mathcal{P}^{vl}(\hat{j})$, are related by the continuity equation (Eq. 10). From the continuity equation, $\mathcal{P}^{vl}(\hat{j})$ is the set of fluxes that

$^{[72]}$In algebraic graph theory, $\mathcal{P}^{sc}(0) = \text{Im} S$ is called cocycle space.

$^{[73]}$In algebraic graph theory, $\mathcal{P}^{vl}(0)$ is called the cycle space.
induce the same velocity as a reference $\hat{j}$ does: $j \in \mathcal{P}^{\text{vl}}(\hat{j}) \iff \dot{x} = -S\hat{j} = -Sj$. Thereby, $\mathcal{P}^{\text{vl}}(\hat{j})$ is parametrized as follows:

$$\mathcal{P}^{\text{vl}}(\dot{x}) = \{ j \in \mathcal{J} | Sj = \dot{x} \}, \quad \dot{x} \in \text{Im}[S] = \text{Ker}[U],$$

(86)

This subspace is crucial to characterize fluxes that can realize the same dynamics as the reference one.

The stoichiometric subspace $\mathcal{P}^{\text{sc}}(x_0)$ determines the subspace in which the dynamics are algebraically constrained via the topology of the underlying graph or hypergraph. Because $\dot{x} = -Sj(x(t))$, for an initial state $x(0) = x_0$, $x(t) - x_0 \in \text{Im}[S]$ should hold, meaning that $x(t) \in \mathcal{P}^{\text{sc}}(x_0)$. Thus, $\mathcal{P}^{\text{sc}}(x_0)$ is the subspace in which the dynamics are restricted by the initial condition $x_0$. $\mathcal{P}^{\text{sc}}(x_0)$ can also be represented parametrically, which provides it with another characterization as the quantities which are conserved by the dynamics. For any vector $u \in \text{Ker}S^T$, $\eta(t) := u^T x(t)$ is constant over time:

$$\dot{\eta}(t) = \frac{du^T x(t)}{dt} = u^T \frac{dx(t)}{dt} = -u^T Sj(x) = 0.$$ 

(87)

In Sec. IIIA, we defined a matrix $U$ by a complete basis of $\text{Ker}S^T$ so that $\text{Im}U^T = \text{Ker}S^T$. Using $U$, the conserved quantities for a given initial condition $x_0$ are obtained as $\eta = Ux_0 = \cup x(t)$. Because $\text{Im}U$ is isomorphic to $C_{-1}(\mathbb{H})$, the stoichiometric subspace is explicitly parametrized by the conserved quantities (an element of $C_{-1}(\mathbb{H})$):

$$\mathcal{P}^{\text{sc}}(\eta) = \{ x \in \mathcal{X} | Ux = \eta \}, \quad \eta \in C_{-1}(\mathbb{H}).$$

(88)

For rMJP, the conserved quantity is reduced to the conservation of probability $1p(t) = 1$ and $\mathcal{P}^{\text{sc}}(p_0)$ becomes the probability simplex. Because $\text{Ker}B^T$ determines the connected components of the graph $G$ and we conventionally assume that the underlying graph is connected in rMJP, we only have the one-dimensional cokernel space and one conserved quantity, which is $\eta = 1$. Thus, the conservation of probability or, equivalently, the restriction of $p$ in the probability simplex is automatically guaranteed from the topological constraint of the dynamics if we start from the initial state satisfying $1^T p_0 = 1$.

The iso-force subspace $\mathcal{P}^{\text{fr}}(f')$ and the equilibrium subspace $\mathcal{P}^{\text{eq}}(y)$ are related to the equilibrium and nonequilibrium force equations, Eq. 55 and Eq. 58. The equilibrium gradient force defined in Eq. 55 satisfies $f(x) \in \text{Im}S^T = \mathcal{P}^{\text{fr}}(0)$. Thus, the gradient-force subspace $\mathcal{P}^{\text{fr}}(0)$ is the set of equilibrium gradient forces. $\mathcal{P}^{\text{fr}}(f')$ is its shift by $f' \in \mathcal{F}_x$. 

46
Thus, for $f' \not\in \mathcal{P}_{fr}(0)$, $\mathcal{P}_{fr}(f')$ is a quotient set of nonequilibrium forces by the equilibrium force $\mathcal{P}_{fr}(0)$. Using $\mathcal{V}$ defined in Sec. III A, we can represent $\mathcal{P}_{fr}$ parametrically as

$$\mathcal{P}_{fr}(\zeta) = \{ f \in \mathcal{F}_x | \mathcal{V}^T f = \zeta \}, \quad \zeta \in C^2(\mathbb{H})$$

(89)

because $\mathcal{F}_x / \text{Im}\mathcal{S}^T \cong \mathcal{F}_x / \text{Ker}\mathcal{V}^T \cong \text{Im}\mathcal{V}^T \cong C^2(\mathbb{H})$. Thus, $\zeta$ characterizes the type of nonequilibrium forces.

Finally, the equilibrium subspace $\mathcal{P}_{eq}(\tilde{x})$ can also be regarded as the set of potentials $y$ that generate the same gradient force because any $y \in \mathcal{P}_{eq}(\tilde{y})$ satisfies $f' = S^T y = S^T \tilde{y} \in \mathcal{P}_{fr}(0)$. Due to this, the equilibrium subspace $\mathcal{P}_{eq}$ is parameterized as

$$\mathcal{P}_{eq}(f') = \{ y \in \mathcal{Y} | S^T y = f' \}, \quad f' \in \text{Im}[S^T].$$

(90)

The parametric forms of the subspaces are summarized as follows:

$$\mathcal{P}_{vl}(\dot{x}) = \{ j \in \mathcal{J}_x | \mathcal{S}j = \dot{x} \}, \quad \dot{x} \in \text{Im}[\mathcal{S}] = \text{Ker}[\mathcal{U}],$$

(91)

$$\mathcal{P}_{sc}(\eta) = \{ x \in \mathcal{X} | \mathcal{U}x = \eta \}, \quad \eta \in \text{Im}[\mathcal{U}] = C_{-1}(\mathbb{H}),$$

(92)

$$\mathcal{P}_{fr}(\zeta) = \{ f \in \mathcal{F}_x | \mathcal{V}^T f = \zeta \}, \quad \zeta \in \text{Im}[\mathcal{V}^T] = C^2(\mathbb{H}),$$

(93)

$$\mathcal{P}_{eq}(f') = \{ y \in \mathcal{Y} | S^T y = f' \}, \quad f' \in \text{Im}[S^T] = \text{Ker}[\mathcal{V}^T].$$

(94)

From these subspaces, we can obtain dual foliations on the vertex and edge spaces.

C. Dual Manifold, Dual Foliation, and Pythagorean relation in vertex spaces

For the subspaces $\mathcal{P}_{sc}$ and $\mathcal{P}_{eq}$ in the vertex spaces, we introduce their Legendre transformation via the thermodynamic functions, $\Phi(x)$ and $\Phi^*(y)$, which form the dual foliation with the orthogonal subspace (Fig. 6, left).

Definition 30 (Stoichiometric manifold in $\mathcal{Y}$ and equilibrium manifold in $\mathcal{X}$). The stoichiometric and equilibrium manifolds (Fig. 6, left) are defined respectively as

$$\mathcal{M}_{sc}(y_0) := \partial \Phi[\mathcal{P}_{sc}(x_0)] \subset \mathcal{Y}, \quad y_0 = \partial \Phi(x_0),$$

(95)

$$\mathcal{M}_{eq}(\bar{x}) := \partial \Phi^*[\mathcal{P}_{eq}(\bar{y})] \subset \mathcal{X}, \quad \bar{x} = \partial \Phi^*(\bar{y}).$$

(96)

Lemma 1 (Dual foliation in vertex space[84]). $\mathcal{P}_{sc}$ and $\mathcal{M}_{sc}$ are foliations of $\mathcal{X}$ and $\mathcal{M}_{eq}$ and $\mathcal{P}_{eq}$ are foliations of $\mathcal{Y}$. For each pair of $(x_0, \bar{x})$, the intersection of $\mathcal{P}_{sc}(x_0)$ and $\mathcal{M}_{eq}(\bar{x})$...
FIG. 6. Diagrammatic representation of the dual foliations in $\mathcal{X}$, $\mathcal{Y}$, $\mathcal{J}_x$, and $\mathcal{F}_x$ spaces.

is unique and transversal. The same applies to $\mathcal{M}^{sc}(y_0)$ and $\mathcal{P}^{eq}(\bar{y})$. Then, $(\mathcal{P}^{sc}, \mathcal{M}^{eq})$ and $(\mathcal{M}^{sc}, \mathcal{P}^{eq})$ form dual foliations (nonlinear coordinate systems) in $\mathcal{X}$ and $\mathcal{Y}$ spaces, respectively.

Proof. The polyhedron $\mathcal{P}^{sc}(x_0)$ and the affine subspace $\mathcal{P}^{eq}(\bar{y})$ can cover the whole $\mathcal{X}$ and $\mathcal{Y}$ by changing $x_0$ and $\bar{y}$, respectively. Similarly, $\mathcal{M}^{eq}(\bar{x})$ and $\mathcal{M}^{sc}(y_0)$ can cover the whole $\mathcal{X}$ and $\mathcal{Y}$ because Legendre transformations by the thermodynamic functions are one-to-one between $\mathcal{X}$ and $\mathcal{Y}$. Consider the intersection of $\mathcal{P}^{sc}(x_0)$ and $\mathcal{M}^{eq}(\bar{x})$ in $\mathcal{X}$ space:

$$x^\dagger := \mathcal{P}^{sc}(x_0) \cap \mathcal{M}^{eq}(\bar{x}).$$

(97)

The existence of $x^\dagger$ is related to the existence of $x^\dagger$ defined by the following convex opti-
mization problem:
\[
x^\dagger := \arg \min_{x \in \mathcal{P}^{sc}(x_0)} D^X[x \| \bar{x}]. \tag{98}
\]

Because of the properties of \(\Phi(x)\), \(D^X[x \| \bar{x}]\) and its linear restriction to \(\mathcal{P}^{sc}(x_0)\) are strictly convex with respect to \(x\). Thus, if \(x^\dagger \in \mathcal{P}^{sc}(x_0)\), \(x^\dagger\) is unique and either satisfies the stationarity condition \(x^\dagger \in \mathcal{P}^{sc}(x_0) \cap \mathcal{M}^{eq}(\bar{x})\) or locates at the boundary if \(x^\dagger \notin \mathcal{P}^{sc}(x_0)\), where we used \(\frac{\partial D^X[x \| \bar{x}]}{\partial x} \mathbb{S} = 0 \iff (y - \bar{y}) \mathbb{S} = 0 \iff y \in \mathcal{P}^{eq}(\bar{y}) \iff x \in \mathcal{M}^{eq}(\bar{x})\). Let \(x_{br} \in \mathbb{R}_{\geq 0}^N \setminus \mathcal{X}\) and \(x_{in} \in \mathcal{X}\) be arbitrary points on the boundary and interior of \(\mathcal{X}\). From the condition Eq. 23 of the thermodynamic function, for \(x^\lambda := \lambda x_{in} + (1 - \lambda)x_{br}\) where \(\lambda \in [0, 1]\),
\[
\lim_{\lambda \to +0} \frac{d D^X[x_\lambda \| \bar{x}]}{d \lambda} = \lim_{\lambda \to +0} \left[ \frac{d \Phi(x_\lambda)}{d \lambda} - \left\langle y, \frac{d x_\lambda}{d \lambda} \right\rangle \right] = -\infty. \tag{99}
\]

Thus, \(x^\dagger \notin \mathcal{X}\) is excluded, and the intersection exists, i.e., \(x^\dagger \in \mathcal{P}^{sc}(x_0) \cap \mathcal{M}^{eq}(\bar{x})\). The intersection \(x^\dagger\) is unique and transversal because, for any \(x_{sc} \in \mathcal{P}^{sc}(x_0)\) and \(x_{eq} \in \mathcal{M}^{eq}(\bar{x})\),
\[
\langle x_{sc} - x^\dagger, y_{eq} - y^\dagger \rangle = 0
\]
holds. The dimensions of \(\mathcal{P}^{sc}(x_0)\) and \(\mathcal{M}^{eq}(\bar{x})\) are complementary, the intersection \(x^\dagger\) is unique. Thus, \(x^\dagger = x^\dagger\). As a result, \(x^\dagger \in \mathcal{P}^{sc}(x_0) \cap \mathcal{M}^{eq}(\bar{x})\) always exists, and \((\mathcal{P}^{X}_{sc}, \mathcal{M}^{X}_{eq})\) forms a dual foliation in \(\mathcal{X}\). Also \((\mathcal{M}^{Y}_{sc}, \mathcal{P}^{Y}_{eq})\) does in \(\mathcal{Y}\) because they are bijective Legendre duals of \((\mathcal{P}^{X}_{sc}, \mathcal{M}^{X}_{eq})\).

This result is reduced to Birch’s theorem[100, 102] and the seminal result by Horn and Jackson[40] when the thermodynamic function is the generalized KL divergence.

With the dual foliation, we can consider the generalized Pythagorean relations and orthogonal decomposition. For any three points satisfying \(x \in \mathcal{P}^{sc}(x_0)\), \(x_q \in \mathcal{M}^{eq}(\bar{x})\), and \(x^\dagger = \mathcal{P}^{sc}(x_0) \cap \mathcal{M}^{eq}(\bar{x})\), we have the generalized Pythagorean relation:
\[
D^X[x \| x_q] = D^X[x \| x^\dagger] + D^X[x^\dagger \| x_q]. \tag{100}
\]

In \(\mathcal{Y}\) space, we also have the dual version of the relations as
\[
D^Y[y_q \| y_p] = D^Y[y_q \| y^\dagger] + D^Y[y^\dagger \| y_p]. \tag{101}
\]

and
\[
y_{eq} = \arg \min_{y_q \in \mathcal{M}^{eq}(y_0)} D^Y[y_q \| y_p] = \arg \min_{y_q \in \mathcal{P}^{eq}(\bar{y})} D^Y[y_q \| y_q] = y^\dagger. \tag{102}
\]

These relations are used to characterize the steady state of equilibrium and nonequilibrium flow geometrically and also variationally.
Remark 8 (Interpretation in terms of statistical inference). The meaning of the equilibrium manifold in statistics can be clarified more explicitly by considering the specific form of thermodynamic function (Eq. 64). For this thermodynamic function, the equilibrium manifold $\mathcal{M}^{eq}(\tilde{\mathbf{p}})$ is represented as

$$\mathcal{M}^{eq}(\tilde{\mathbf{p}}) = \{ \mathbf{p} \in \mathcal{X} | \ln \mathbf{p} - \ln \tilde{\mathbf{p}} \in \ker \mathbf{S}^T \} = \{ \mathbf{p} \in \mathcal{X} | \mathbf{p} = \tilde{\mathbf{p}} \circ \exp \left[ \mathbf{U}^T \eta^* \right], \eta^* \in C^{-1}(\mathbb{H}) \}$$

(103)

where we use the fact $\mathbf{S}^T \mathbf{U}^T = 0$. Thus, $\mathcal{M}^{eq}(\tilde{\mathbf{p}})$ is the exponential family with algebraic constraints via $\mathbf{U}^T$. In contrast, $\mathcal{P}^{sc}(\eta)$ can be regarded as the data manifold, which constrains $\mathbf{p}$ by $\eta = \mathbf{U} \mathbf{p}$, because $\mathbf{U} \mathbf{p}$ can be interpreted as expectation of observables $\{ \mathbf{u}_t \}_{t \in [1, N]}$. Thus, the intersection $\mathbf{p}^* = \mathcal{P}^{sc}(\eta) \cap \mathcal{M}^{eq}(\tilde{\mathbf{p}})$ is the maximum likelihood estimator. The exponential family with linear algebraic constraints as in Eq. 103 appears in algebraic statistics where $\mathbf{U}$ is sometimes called the design matrix[102][74].

D. Dual manifold, dual foliation in edge spaces and generalized Helmholtz-Hodge-Kodaira decomposition

For the edge spaces, we similarly introduce the iso-velocity and iso-force manifolds, which are the duals of $\mathcal{P}^{fr}(\mathbf{f}')$ and $\mathcal{P}^{vl}(\hat{\mathbf{j}})$, respectively, via the Legendre transformation of the dissipation functions, $\Psi_x(\mathbf{j})$ and $\Psi^*_x(\mathbf{f})$ (Fig. 6, right):

**Definition 31** (Iso-velocity manifold in $\mathcal{F}_x$ and iso-force manifold in $\mathcal{J}_x$). The iso-velocity and iso-force manifolds (Fig. 6, right) are defined as follows:

\[
\mathcal{M}^{vl}_{x}(\hat{\mathbf{f}}) := \partial \Psi_x[\mathcal{P}^{vl}(\hat{\mathbf{j}})] \subset \mathcal{F}_x, \quad \hat{\mathbf{f}} = \partial \Psi_x(\hat{\mathbf{j}}), \tag{104}
\]

\[
\mathcal{M}^{fr}_{x}(\mathbf{j}') := \partial \Psi^*_x[\mathcal{P}^{fr}(\mathbf{f}')] \subset \mathcal{J}_x, \quad \mathbf{j}' = \partial \Psi^*_x(\mathbf{f}'). \tag{105}
\]

It should be noted that $\mathcal{M}^{vl}_{x}(\hat{\mathbf{f}})$ and $\mathcal{M}^{fr}_{x}(\mathbf{j}')$ are dependent on $\mathbf{x}$ via the $\mathbf{x}$ dependence of the dissipation functions. We obtain the intersections in $\mathcal{J}_x$ and $\mathcal{F}_x$:

\[
\mathbf{j}^\dagger := \mathcal{P}^{vl}(\hat{\mathbf{j}}) \cap \mathcal{M}^{fr}_{x}(\mathbf{j}'), \quad \mathbf{f}^\dagger := \mathcal{M}^{vl}_{x}(\hat{\mathbf{f}}) \cap \mathcal{P}^{fr}(\mathbf{f}'), \tag{106}
\]

[74] In algebraic statistics, $\mathbf{U}$ is explicitly given as constraints of a statistical model. In the dynamics on graph and hypergraph, $\mathbf{S}$ is explicitly given, and $\mathbf{U}$ is implicitly defined as a complete basis of $\ker \mathbf{S}^T$. As a result, their connection is not apparently obvious.
which are also unique and transversal for each fixed \( x \in \mathcal{X} \) because \( J_x \) and \( F_x \) are whole vector spaces and the Legendre transformation are one-to-one. Thus, similarly to the case of vertex space, we have the dual foliation:

**Lemma 2** (Dual foliation in edge space[82]). For each \( x \in X \), \((P^v, M^f_x)\) and \((M^v_x, P^f)\) form dual foliations in \( J_x \) and \( F_x \) spaces, respectively.

For \( \hat{j} \) and \( f' \), and their intersections \( j^\dagger \) and \( f^\dagger \) defined in Eq. 106, \( \langle \hat{j} - j^\dagger, f^\dagger - f' \rangle = 0 \) holds. Thus, we have the generalized Pythagorean relations:

\[
\mathcal{D}^J_x[j||j'] = \mathcal{D}^J_x[\hat{j}||j^\dagger] + \mathcal{D}^J_x[j^\dagger||j'],
\mathcal{D}^F_x[f'; \hat{f}] = \mathcal{D}^F_x[f'||f^\dagger] + \mathcal{D}^F_x[f^\dagger; \hat{f}].
\tag{107}
\]

In contrast to the thermodynamic functions \((\Phi, \Phi^*)\), the dissipation functions have symmetry, which makes the origins 0 in \( J_x \) and \( F_x \) special and leads to the generalized Helmholtz-Hodge-Kodaira decomposition.

**Theorem 1** (Generalized Helmholtz-Hodge-Kodaira (HHK) decomposition[82]). For a given flux-force Legendre pair \((j, f)\) \( \in (J_x, F_x) \), we have their unique \( x \)-dependent decompositions:

\[
j = j_{eq}(x) + (j - j_{eq}(x)), \quad f = f_{st}(x) + (f - f_{st}(x)),
\tag{108}
\]

such that \( f_{eq}(x) \in P^f(0) \), \( j - j_{eq}(x) \in P^v(0) \), \( f - f_{st}(x) \in P^f(0) \), and \( j_{st}(x) \in P^v(0) \) hold. \( j_{eq}(x) \) and \( f_{st}(x) \) are characterized geometrically as

\[
j_{eq}(x) := P^v(j) \cap M^f_x(0), \quad f_{st}(x) := M^v_x(0) \cap P^f(f).
\tag{109}
\]

Furthermore, \( j_{eq} \) and \( f_{st} \) are also characterized variationally as the minimizers of dissipation functions:

\[
j_{eq}(x) = \arg \min_{j' \in P^v(j)} \Psi_x(j'), \quad f_{st}(x) = \arg \min_{f'' \in P^f(f)} \Psi^*_x(f'').
\tag{110}
\]

**Proof.** The uniqueness of \( j_{eq}(x) \) and \( f_{st}(x) \) as intersections in Eq. 109 follows immediately from the property of the dual foliations. Because, for any \( j' \in P^v(j) \) and \( f'' \in P^f(f) \), \( \langle j' - j_{eq}, f_{eq} \rangle = 0 \) and \( \langle j_{st}, f'' - f_{st} \rangle = 0 \) hold, the generalized Pythagorean relations lead to

\[
\mathcal{D}^J_x[j'||j_{eq}; 0] = \mathcal{D}^J_x[j'||j_{eq}]+\mathcal{D}^J_x[j_{eq}; 0], \quad \mathcal{D}^F_x[f''||f_{st}; 0] = \mathcal{D}^F_x[f''||f_{st}]+\mathcal{D}^F_x[f_{st}; 0].
\]
Because $D_x^T[j';0] = \Psi_x(j')$ and $D_x^T[f'';0] = \Psi_x^{*}(f'')$ hold, the relations are reduced to

$$\Psi_x(j') = D_x^T[j'|j_{eq}] + \Psi_x(j_{eq}), \quad \Psi_x^{*}(f'') = D_x^T[f''|f_{st}] + \Psi_x^{*}(f_{st}).$$

(111)

Then Eq. 110 follows.

The decomposed flux $j_{eq}$ and force $f_{st}$ play a particularly important role in dynamics. From the definition, $j_{eq}$ is the gradient flux (the flux whose corresponding force $f_{eq}$ is an equilibrium gradient force, i.e. $f_{eq} \in \mathcal{P}^fr(0) = \text{Im}S^T = \text{Im}[\text{grad}_{\mathcal{S}}]$), which induces the same instantaneous velocity $\dot{x}$ as $j$ does, i.e., $\dot{x} = -\text{div}_S j = -\text{div}_S j_{eq}$. Thus, $j_{eq}$ is the gradient flux mimicking the dynamics of the nonequilibrium flux $j$. This gradient flux is uniquely determined owing to the information-geometric orthogonality of $\mathcal{P}^{st}(j)$ and $\mathcal{M}_x^{fr}(0)$. Moreover, the decomposition $j = j_{eq} + (j - j_{eq})$ can be regarded as an information-geometric generalization of the Helmholtz-Hodge-Kodaira decomposition in vector calculus, because $(j - j_{eq})$ is divergence free, i.e., $\text{div}_S (j - j_{eq}) = 0$, and $f_{eq}$ is a curl-free gradient force, i.e., $f_{eq} \in \mathcal{P}^fr(0) = \text{Im}[S^T] = \text{Ker}[V^T]$.

On the contrary, by definition, $j_{st} \in \mathcal{P}^{st}(0)$ is the flux that makes the state $x$ a steady state, i.e., $\dot{x} = 0$, and is also induced by the force in the same quotient set of force $\mathcal{P}^{fr}(f)$ as $f$. The decomposition $f = f_{st} + (f - f_{st})$ is also a HHK decomposition because $j_{st} \in \mathcal{P}^{st}(0)$ is divergence free, i.e., $\text{div}_S j_{st} = 0$, and $f - f_{st}$ is a curl-free gradient force, i.e., $f - f_{st} \in \mathcal{P}^{fr}(0) = \text{Im}[\text{grad}_{\mathcal{S}}] = \text{Ker}[V^T]$. These decompositions are used in the subsequent sections (Sec. VIII and Sec. VIII).

VII. CENTRAL AFFINE MANIFOLD AND HILBERT ORTHOGONALITY

The dual foliation is an essential geometric object in information geometry. While less common than the dual foliation, the central affine manifold defined by a convex function also plays integral roles in information geometry[147].

[77] It should be noted that, in general, $j_{st} \neq j - j_{eq}$ and $f_{eq} \neq f - f_{st}$ and as a result $j \neq j_{eq} + j_{st}$ and $j \neq f_{eq} + f_{st}$ due to the nonlinearity of Legendre transformation, except when the dissipation functions are quadratic under which the Legendre dual relation is reduced to the linear inner-product relation.
Definition 32 (Central affine manifolds in $J_x$ and $F_x$). The central affine manifolds in $J_x$ and $F_x$ are defined as the level sets of $\Psi_x(j)$ and $\Psi^*_x(f)$, respectively:

$$
C^\Psi_x(c) := \{j|\Psi_x(j) = c\} \subset J_x, \quad C^{\Psi^*}_x(c) := \{f|\Psi^*_x(f) = c\} \subset F_x,
$$

where $c \in \mathbb{R}_{\geq 0}$. For a given $j' \in J_x$ or $f' \in F_x$, the manifolds are also denoted as

$$
C^\Psi_x(j') := \{j|\Psi_x(j) = \Psi_x(j')\}, \quad C^{\Psi^*}_x(f') := \{f|\Psi^*_x(f) = \Psi^*_x(f')\}.
$$

Their Legendre transformations are also called (dual) central affine manifolds:

$$
M^{\Psi}_x(c) := \partial \Psi_x[C^\Psi_x(c)] \subset F_x, \quad M^{\Psi^*}_x(c) := \partial \Psi^*_x[C^{\Psi^*}_x(c)] \subset J_x.
$$

A. Pseudo-Hilbert-isosceles orthogonality and decomposition

By employing the central affine manifold, we can introduce another type of generalized orthogonality:

Definition 33 (Pseudo-Hilbert-isosceles orthogonality[77, 78, 80]). Pseudo-Hilbert-isosceles orthogonality between $j_S, j_A \in J_x$ and between $f_S, f_A \in F_x$ are defined as follows:

$$
\begin{align*}
&j_S \perp_H j_A \iff \Psi_x(j_S + j_A) = \Psi_x(j_S - j_A) \quad (115) \\
&f_S \perp_H f_A \iff \Psi^*_x(f_S + f_A) = \Psi^*_x(f_S - f_A). \quad (116)
\end{align*}
$$

This orthogonality is motivated by the relation $\|j_S + j_A\|^2 = \|j_S - j_A\|^2$ satisfied by an orthogonal pair $j_S \perp j_A$ under a usual inner product structure and its induced norm $\|\cdot\|^2$[77]. By employing this orthogonality, we obtain a pseudo-Hilbert isosceles decomposition $j$ as follows:

---

[76] While we introduce the central affine manifolds only on the edge space, they can be defined on the vertex space as well. The central affine manifolds on the vertex space become fundamental when we work on the isobaric processes in which the volume changes in conjunction with the reactions[85]. In this case, the volume is a global variable affecting all the reactions simultaneously.

[77] If $\|\cdot\|^2$ is a squared norm that is not necessarily induced from an inner product, the orthogonality is called isosceles or James orthogonality[149]. Here, we further replace $\|\cdot\|^2$ with the dissipation function, which does not satisfy some conditions required to be a norm. Thus, we call the decomposition pseudo-Hilbert isosceles.
Lemma 3 (A positive decomposition of the bilinear pairing via pseudo-Hilbert-isosceles orthogonality [77, 78, 80, 82]). For a given \( j \in J_x \) and any \( j' \) on the same central affine manifold as \( j \), i.e., \( j' \in C_x^\psi(j) \), we obtain the Pseudo-Hilbert-isosceles orthogonal decomposition \( j = j_S + j_A \):

\[
    j_S := \frac{1}{2}(j + j'), \quad j_A := \frac{1}{2}(j - j'),
\]

(117)

where \( j_S \perp_H j_A \) and \( j' = j_S - j_A \) hold. In addition, this decomposition induces a positive decomposition of the bilinear product \( \langle j, f \rangle = \langle j_S, f \rangle + \langle j_A, f \rangle \) where

\[
    \langle j_S, f \rangle = \frac{1}{2}D_x^{\mathcal{J}, \mathcal{F}}[j || f] \geq 0, \quad \langle j_A, f \rangle = \frac{1}{2}D_x^{\mathcal{J}, \mathcal{F}}[j || f] \geq 0,
\]

(118)

hold. Similarly, for \( f \in \mathcal{F}_x \) and \( f'' \in C_x^{\psi'}(f) \), the positive orthogonal decomposition \( f = f_S + f_A \) is obtained by \( f_S := \frac{1}{2}(f + f'') \), and \( f_A := \frac{1}{2}(f - f'') \) and the associated relations:

\[
    \langle j, f_A \rangle = \frac{1}{2}D_x^{\mathcal{J}, \mathcal{F}}[j || f''] \geq 0, \quad \langle j, f_S \rangle = \frac{1}{2}D_x^{\mathcal{J}, \mathcal{F}}[j || f''] \geq 0,
\]

(119)

hold.

These decompositions were introduced in [77] for MJP and extended to CRN in [78, 80], whereas we pointed out its information geometric aspect in [82]. The decomposition plays the role of characterizing the gradient-flow-like property of non-gradient flows.

VIII. INFORMATION-GEOMETRIC PROPERTIES OF EQUILIBRIUM GRADIENT FLOW

In this section, we describe several properties of the equilibrium flow (Eq. 56) from the viewpoint of information geometry by employing the objects introduced in the previous sections. Such properties include the existence and uniqueness of the steady state (static property), convergence to the state (kinetic property), and the balance between information-geometric quantities associated with the steady state and convergence along the trajectory (the connection between static and kinetic properties). These properties are consistent with those that thermodynamic equilibrium systems should have. In addition, several results are extensions of the results obtained for FPE in the context of functional analysis, in the theories of partial differential equations, and optimal transport.
A. Properties of equilibrium flow

The following property of the equilibrium state characterizes the static aspect of the equilibrium flow and is fundamentally ascribed to the dually flat structure of vertex spaces\cite{78}:

**Proposition 6** (Equilibrium state and its geometric and variational characterizations). The steady state of the equilibrium flow $x_t$ (Eq. 56) starting from $x(0) = x_0$ is called the equilibrium state $x_{eq}$. For each $x_0$, the equilibrium state is identical to the intersection $x^\dagger = P^{sc}(x_0) \cap M^{eq}(\tilde{x})$, i.e., $x_{eq} = x^\dagger$, and thus uniquely exists for a given pair of the initial state $x_0$ and the parameter of equilibrium flow $\tilde{x}$. The equilibrium state $x_{eq}$ is also characterized variationally as

$$x_{eq} = \arg \min_{x \in P^{sc}(x_0)} D^X_\Phi[x \parallel x_0] = \arg \min_{x_q \in M^{eq}(\tilde{x})} D^X_\Phi[x_0 \parallel x_q]. \quad (120)$$

Moreover, $M^{eq}(\tilde{x}) = M^{DB}$ holds.

**Proof.** From Prop. 23, $x_{eq} \in M^{DB}$, from which $f(x_{eq}) = 0$ follows. For the equilibrium force (Eq. 55), $M^{DB} = \{x \mid f(x) = 0\} = \{x \mid S^T(\partial \Phi[x] - \partial \Phi[\tilde{x}]) = 0\} = M^{eq}(\tilde{x})$ holds. Thus, $x_{eq} \in M^{eq}(\tilde{x})$. Because the initial state is $x_0$, $x_{eq} \in P^{sc}(x_0)$. Thus, $x_{eq} = x^\dagger = P^{sc}(x_0) \cap M^{eq}(\tilde{x})$. The first equality of Eq. 120 is obvious from the proof of the dual foliation (Lemma 1). The second equality is from the generalized Pythagorean relation (Eq. 100).

The second property is kinetic in nature and characterizes the Bregman divergence as the generalized driving potential, which ensures the convergence of $x_t$ to the equilibrium state. This property is attributed to the second dually flat structure on the edge spaces.

**Proposition 7** (Bregman divergence and Gibb's H-Theorem). For the trajectory of the equilibrium flow $x_t$ (Eq. 56) starting from $x(0) = x_0$, the thermodynamic function $D^X_\Phi[x_t \parallel \tilde{x}]$ decreases, that is, $dD^X_\Phi[x_t \parallel \tilde{x}] / dt < 0$ except at $x_t \in M^{eq}(\tilde{x})$ where $dD^X_\Phi[x_t \parallel \tilde{x}] / dt = 0$ holds. Thus, the equilibrium state $x_{eq} \in P^{sc}(x_0) \cap M^{eq}(\tilde{x})$ is locally and asymptotically stable.

**Proof.** By replacing $F(x)$ in Prop. 3 with $D^X_\Phi[x \parallel \tilde{x}]$, we obtain $dD^X_\Phi[x_t \parallel \tilde{x}] / dt = -\left[\Psi_{x_t}^*(f(x_t)) + \Psi_{x_t}(j(x_t))\right] \leq 0$ and the equality holds if and only if $f(x_t) = 0 \Leftrightarrow x_t \in M^{eq}(\tilde{x})$.

\cite{78} Actually, this result is independent of the detail of the dissipation functions.
Because $D^{X}_\Phi [x\|\tilde{x}]$ can be identified with the difference of total entropy between $x$ and $\tilde{x}$ for thermodynamic systems such as CRN[47], $dD^{X}_\Phi [x_t\|\tilde{x}_{eq}]/dt \leq 0$ corresponds to the nondecreasing property of thermodynamic entropy, which is also referred as Gibb’s H-theorem[79].

The third property provides a connection between the thermodynamic function and the dissipation function, which is immediately obtained from the De Giorgi’s formulation of the generalized gradient flow (Eq. 50):

**Proposition 8** (Balancing of thermodynamic function and dissipation function). For the trajectory of the equilibrium flow $x_t$ (Eq. 56) starting from $x(0) = x_0$, the following relation holds for the thermodynamic function and the dissipation function:

$$D^{X}_\Phi [x_0\|\tilde{x}] - D^{X}_\Phi [x_t\|\tilde{x}] = \int_{t'=0}^{t} \left[ \psi_{\omega(x_{t'})}(f(x_{t'})) + \psi_{\omega(x_{t'})}(j(x_{t'})) \right] dt = \int_{t'=0}^{t} \dot{\Sigma} dt, \quad (121)$$

In physics and chemistry, this relation means that the difference in the thermodynamic (potential) function between $x_t$ and $x_0$ (the left-hand side), i.e., the change in total entropy, is equal to the integral of dissipation along $x_t$ (the right-hand side), i.e., the entropy production, for equilibrium systems.

All these results indicate that the equilibrium flow and its properties mathematically abstract the properties of physical equilibrium systems. The equilibrium state $x_{eq}$ is characterized algebraically by the unique intersection of $\mathcal{P}^{sc}(x_0)$ and $\mathcal{M}^{eq}(\tilde{x})$ and also variationally by Eq. 120. The convergence to $x_{eq}$ is guaranteed by $dD^{X}_\Phi [x_t\|$ $\tilde{x}]/dt \leq 0$. Furthermore, the entropy-dissipation balance relation (Eq. 121) itself defines the equilibrium system abstractly as the De Giorgi’s formulation (Eq. 50) does.

**B. Induced dually flat structure on tangent-cotangent spaces as a generalized Otto structure**

The equilibrium state is characterized geometrically and variationally via the information-geometric structure on the vertex spaces ($\mathcal{X}$, $\mathcal{Y}$) as in Prop. 6. Similarly, the flux (kinetic

[79] We have multiple types of H-theorems. The most famous one is Boltzmann’s H theorem, in which the H function is derived from the microscopic dynamics of a system. In Gibb’s H-theorem, H fun-
Induced structure on tangent -cotangent spaces
\[ \tilde{T}_x^* \mathcal{X} \cup \mathcal{U} \rightarrow f^\dagger(x, \nu) = f^\dagger(u) \]

\[ \partial \Psi_x \uparrow \partial \tilde{\Psi}_x \]
\[ v \leftarrow j^\dagger(x, \nu) = j^\dagger(x, u) \]
\[ \tilde{T}_x \mathcal{X} \quad \mathcal{P}^{vl}(\nu) \cap \mathcal{M}^{fr}(0) \]

Induced structure on cycle spaces
\[ \mathcal{M}^{vl}(0) \cap \mathcal{P}^{fr}(\zeta) \quad \mathcal{M}^{vl}(0) \cap \mathcal{P}^{fr}(\zeta) \]
\[ \partial \Psi_x \uparrow \partial \Psi_x \]
\[ j^\diamond(x, \zeta) = j^\diamond(z) \]
\[ \mathcal{X} \leftarrow \tilde{T}_x \mathcal{X} \quad \mathcal{M}^{fr}(0) \quad \mathcal{J}_x \]

FIG. 7. (a) The induced dually flat structure on the restricted tangent and cotangent spaces from the dissipation functions on the edge spaces. (b) The relationship of the induced dually flat structure in (a) with the Fisher information matrices induced from the thermodynamic functions. (c) The induced dually flat structure on the cycle spaces from the dissipation functions on the edge spaces.

Lemma 4 (Gradient force as the minimizer of primal dissipation). For a given trajectory \( \{x_t\} \), we define the trajectory of the flux \( \{j^\dagger_t\} \) minimizing the primal dissipation:

\[ \{j^\dagger_t\} := \arg \min_{\{j_t\}} \int_0^t \Psi_{x,t}[j_{t'}] dt', \quad \text{s.t.} \quad \dot{x}_t + \text{div}_x j_t = 0 \text{ for all } t' \in [0, t]. \quad (122) \]

Then, \( j^\dagger_t \) is generated by the gradient force, \( f^\dagger_t = \partial \Psi_x[j^\dagger_t] \in \mathcal{P}^{fr}(0) \). Thus, the minimum primal dissipation flux that generates the given \( \{x_t\} \) is the equilibrium flux.

Proof. Because the minimization of Eq. 122 can be conducted pointwise manner for each
\[ t' \in [0, t] \text{ and } \dot{x}_{\nu} + \text{div}_{\mathcal{S}} j_{\nu} = 0 \iff j_{\nu} \in \mathcal{P}^{st}(\dot{x}_{\nu}) \text{, we have} \]

\[ j_{\nu}^{\dagger} = j^{\dagger}(x_{\nu}, \dot{x}_{\nu}) = \arg \min_{j \in \mathcal{P}^{st}(\dot{x}_{\nu})} \Psi_{x_{\nu}}[j] = \mathcal{P}^{st}(\dot{x}_{\nu}) \cap M_{x_{\nu}}^{fr}(0), \]  

(123)

where we used Eq. 109 and Eq. 110. Thus, from \( j_{\nu}^{\dagger} \in M_{x_{\nu}}^{fr}(0) \iff f_{\nu}^{\dagger} \in \mathcal{P}^{fr}(0) \), the minimum dissipation flux \( \{ j_{\nu}^{\dagger} \} \) is generated by the gradient force, \( \{ f_{\nu}^{\dagger} \} = \{ f^{\dagger}(x_{\nu}, \dot{x}_{\nu}) \} \in \mathcal{P}^{fr}(0) \) where \( f^{\dagger}(x, \dot{x}) := \partial \Psi_{x}[j^{\dagger}(x, \dot{x})] \).

By exploiting this unique pairing between \( \dot{x}_{\nu} \) and \( j_{\nu}^{\dagger} \) or \( \dot{x}_{\nu} \) and \( f_{\nu}^{\dagger} \), we can obtain an induced dually flat structure on the restricted tangent and cotangent spaces of \( \mathcal{X} \) and \( \mathcal{Y} \) (Fig. 7 (a)), which can be regarded as an extension of the Otto structure.

**Theorem 2** (Induced dually flat structure on tangent and cotangent spaces). Let \( \tilde{T}_{x} \mathcal{X} := \text{Im} \mathcal{S} \cong \mathcal{P}^{sc}(0) \subset T_{x} \mathcal{X} \) and \( \tilde{T}_{x}^{*} \mathcal{X} := \mathcal{Y}/\text{Ker} \mathcal{S}^{T} \subset T_{x} \mathcal{X} \) be tangent and cotangent spaces on \( \mathcal{X} \) restricted by \( \mathcal{S} \). On \( \tilde{T}_{x} \mathcal{X} \) and \( \tilde{T}_{x}^{*} \mathcal{X} \), we have the Legendre conjugate dissipation functions \( \tilde{\Psi}_{x} : \tilde{T}_{x} \mathcal{X} \to \mathbb{R} \) and \( \tilde{\Psi}_{x}^{*} : \tilde{T}_{x}^{*} \mathcal{X} \to \mathbb{R} \) induced by the dissipation functions on the edge spaces (Fig. 7 (a)).

**Proof.** By employing Eq. 123, for each \( v \in \tilde{T}_{x} \mathcal{X} \), we can uniquely determine \( j^{\dagger}(x, v) \), \( f^{\dagger}(x, v) \in \mathcal{P}^{fr}(0) \), and \( u^{\dagger}(x, v) := -(\mathcal{S}^{T})^{+}f^{\dagger}(x, v) \in \tilde{T}_{x}^{*} \mathcal{X} \), where \( (\mathcal{S}^{T})^{+} : \mathcal{P}^{fr}(0) \to \tilde{T}_{x}^{*} \mathcal{X} \) is the pseudo-inverse of \( \mathcal{S}^{T}[80] \). They satisfy

\[ v = -\mathcal{S} j^{\dagger}(x, v), \quad j^{\dagger}(x, v) = \partial \tilde{\Psi}_{x}^{*}[f^{\dagger}(x, v)], \quad f^{\dagger}(x, v) = -\mathcal{S}^{T} u^{\dagger}(x, v). \]  

(124)

Conversely, for a given \( u \in \tilde{T}_{x}^{*} \mathcal{X} \), we have \( f^{\dagger}(u) \), \( j^{\dagger}(x, u) \), and \( v^{\dagger}(x, u) \) as follows:

\[ v^{\dagger}(x, u) = -\mathcal{S} j^{\dagger}(x, u), \quad j^{\dagger}(x, u) = \partial \tilde{\Psi}_{x}^{*}[f^{\dagger}(u)], \quad f^{\dagger}(u) = -\mathcal{S}^{T} u. \]  

(125)

Thus, for a pair of \((v, u)_{x}\) satisfying \( u = u^{\dagger}(x, v) \), \( v = v^{\dagger}(x, u) \), \( j^{\dagger}(x, v) = j^{\dagger}(x, u) \), and \( f^{\dagger}(x, v) = f^{\dagger}(x, u) \) hold. This pairing establishes a bijection between \( \tilde{T}_{x} \mathcal{X} \) and \( \tilde{T}_{x}^{*} \mathcal{X} \). This bijection is realized by the Legendre transformations of the following induced dissipation functions on \( \tilde{T}_{x} \mathcal{X} \) and \( \tilde{T}_{x}^{*} \mathcal{X} \):

\[ \tilde{\Psi}_{x}(v) := \Psi_{x}(j^{\dagger}(x, v)), \quad \tilde{\Psi}_{x}^{*}(u) := \Psi_{x}^{*}(f^{\dagger}(u)). \]  

(126)

---

[80] Because \( f^{\dagger}(x, v) \in \mathcal{P}^{fr}(0) = \text{Im} \mathcal{S}^{T} \) and \( \tilde{T}_{x} \mathcal{X} := \mathcal{Y}/\text{Ker} \mathcal{S}^{T} \), \( (\mathcal{S}^{T})^{+} \) is uniquely determined.
These functions are Legendre conjugate as follows:

\[
\max_{u' \in \mathcal{T}_x^*} \left[ \langle v, u' \rangle - \tilde{\Psi}_x^*(u') \right] = \max_{u' \in \mathcal{T}_x^*} \left[ \langle -\mathcal{S} j, u' \rangle - \tilde{\Psi}_x^*(u') \right] = \max_{u' \in \mathcal{T}_x^*} \left[ \langle j, -\mathcal{S}^T u' \rangle - \Psi_x^*(-\mathcal{S}^T u') \right]
\]

\[
= \max_{j' \in \mathcal{P}^{fr}(0)} \left[ \langle j, f' \rangle - \Psi_x^*(f') \right] = \max_{j' \in \mathcal{P}^{fr}(0)} \left[ \langle j^\dagger(x, v), f' \rangle - \Psi_x^*(f') + \langle (j - j^\dagger(x, v)), f' \rangle \right]
\]

\[
= \max_{j' \in \mathcal{P}^{fr}(0)} \left[ \langle j^\dagger(x, v), f' \rangle - \Psi_x^*(f') \right] = \Psi_x(j^\dagger(x, v)) = \tilde{\Psi}_x(v),
\]

where we used \( \langle j - j^\dagger(x, v), f' \rangle = 0 \) because \( f' \in \mathcal{P}^{fr}(0) = \text{Im} \mathcal{S}^T \) and \( (j - j^\dagger(x, v)) \in \text{Ker} \mathcal{S} \).

The inverse is also shown:

\[
\max_{v' \in \mathcal{T}_x^*} \left[ \langle v', u \rangle - \tilde{\Psi}_x(v') \right] = \max_{v' \in \mathcal{T}_x^*} \left[ \langle -\mathcal{S} j^\dagger(x, v'), u \rangle - \Psi_x(j^\dagger(x, v')) \right]
\]

\[
= \max_{j^\dagger \in \mathcal{M}_x^f(0)} \left[ \langle j^\dagger, -\mathcal{S}^T u \rangle - \Psi_x(j^\dagger) \right] = \max_{j^\dagger \in \mathcal{M}_x^f(0)} \left[ \langle j^\dagger, f^\dagger(u) \rangle - \Psi_x(j^\dagger) \right]
\]

\[
= \Psi_x^*(f^\dagger(u)) = \tilde{\Psi}_x^*(u),
\]

where we used the fact that \( \{j^\dagger(x, v')\}_{v' \in \mathcal{T}_x^*} = \mathcal{M}_x^{fr} \) in the second line. The pair \((v, u)_x\) are Legendre dual of these functions:

\[
\partial_v \tilde{\Psi}_x(v) = \left[ \frac{\partial j^\dagger(x, v)}{\partial v} \right]^T \frac{\partial \Psi_x(j)}{\partial j} \bigg|_{j = j^\dagger(x, v)} = \left[ \frac{\partial j^\dagger(x, v)}{\partial v} \right]^T f^\dagger(x, v) \tag{127}
\]

\[
= - \left[ \frac{\partial j^\dagger(x, v)}{\partial v} \right]^T \mathcal{S}^T u^\dagger(x, v) = u, \tag{128}
\]

\[
\partial_u \tilde{\Psi}_x^*(u) = \left[ \frac{\partial f^\dagger(u)}{\partial u} \right]^T \frac{\partial \Psi_x^*(f)}{\partial f} \bigg|_{f = f^\dagger(u)} = \left[ \frac{\partial f^\dagger(u)}{\partial u} \right]^T j^\dagger(x, u), \tag{129}
\]

\[
= - \mathcal{S} j^\dagger(x, u) = v, \tag{130}
\]

where we used \( \frac{\partial j^\dagger(x, v)}{\partial v} \mathcal{S}^T = -I \) from \( \frac{\partial}{\partial v} [v + \mathcal{S} j^\dagger(x, v)] = I + \mathcal{S} \frac{\partial j^\dagger(x, v)}{\partial v} \mathcal{S}^T = 0 \) and \( \frac{\partial f^\dagger(u)}{\partial u} = -\mathcal{S}^T \).

They are dissipation functions: strict convexity and 1-coercivity follow from those of the original dissipation functions. Also, we have

\[
(\text{Symmetry}) \quad \tilde{\Psi}_x(-v) = \Psi_x(j^\dagger(x, -v)) = \Psi_x(-j^\dagger(x, v)) = \tilde{\Psi}_x(v) \tag{131}
\]

(Bounded by 0 at 0) \( \tilde{\Psi}_x(v = 0) = \Psi_x(j^\dagger(x, 0)) = \Psi_x(0) = 0. \tag{132} \)
Using the induced dissipation functions, we define the Bregman divergence on $(\tilde{T}_x X, \tilde{T}_x^* X)$, which is associated with the Bregman divergence on $(J_x, F_x)$:
\[
D_{\tilde{\Psi}_x}^{X,Y}[v\|u'] := \tilde{\Psi}_x(v) + \tilde{\Psi}_x^*(u') - \langle v, u' \rangle \tag{133}
\]
\[
= \Psi_x(j^\dagger) + \Psi_x^*(f'^\dagger) - \langle j^\dagger, f'^\dagger \rangle = D_{J_x,F_x}^x[j\|f'^\dagger], \tag{134}
\]
where $j^\dagger = j^\dagger(x, v)$ and $f'^\dagger = f'^\dagger(x, u')$. Therefore, we have the induced dually flat structure on $(\tilde{T}_x X, \tilde{T}_x^* X)$. This induced structure can be regarded as a generalization to discrete manifolds of the Otto structure\cite{64,65}: the formal Riemannian structure induced by the $L^2$-Wasserstein distance. This is also related to Pistone’s infinite-dimensional information geometry\cite{71,123}.

C. Fisher information, natural gradient, mirror descent, evolutionary computation, and optimal transport

In information geometry, it is conventional to use the Fisher information matrices, i.e., the Hessian matrices $G_x$ and $G_y^*$ (Eq. 29) as the metric tensor (Fisher–Rao metric) on $(\mathcal{T}_x \mathcal{X}, \mathcal{T}_x^* \mathcal{X})$ or equivalently on $(\mathcal{T}_y \mathcal{Y}, \mathcal{T}_y^* \mathcal{Y})$ (Fig. 7 (b)). Gradient systems have been defined information-geometrically\cite{24} as a Riemannian gradient flow using the Bregman divergence and the Fisher information matrix of $\Phi(x)$ as the gradient function and the metric tensor, respectively: $\dot{x} = -G_x^{-1}\partial D_\Phi^x[x\|\hat{x}]$. Because both $G_x$ and $D_\Phi^x$ are derived from $\Phi(x)$, this gradient flow becomes a geodesic in $\mathcal{Y}$ space: $\dot{y} = -(y - \hat{y})$. In natural gradient descent\cite{66,68,150}, the Fisher information matrix is used to find the steepest descent gradient of a function $F(\theta)$ on a parameter space $\Theta$ as $\dot{\theta} = -G_\theta^{-1}\partial F(\theta)$, where $G_\theta$ is determined independently of $F(\theta)$ by considering the underlying model parameter space. In optimization, the natural gradient is fundamental in information-geometric optimization algorithms, which contain various evolutionary optimization schemes\cite{69}. In relation to machine learning, the mirror descent is identified with the natural gradient descent by a naive continuous limit\cite{68,151}. Furthermore, optimal transport has recently been employed to replace or integrate the Fisher-Rao metric with the Wasserstein metrics\cite{152,153}. Because the Wasserstein metric can take the underlying manifold information into account, their integration may provide more amenable ways to accommodate various prior and structural information.
The doubly dual flat structure introduced in this work actually provides a solution to generalize those results and the associated problems. The base space $\mathcal{X}$ with the dually flat structure and the associated Fisher information matrix accommodates the conventional natural gradient. The graph or hypergraph structure endows the additional topological relation to the base space of $\mathcal{X}$. The dissipation functions on the edge spaces or their induced versions bestow a more flexible way than the Fisher-Rao metric to represent the loss of the potential function, i.e., the dissipation, at each point in the state space. Upon necessity, we may combine both of them (Fig. 7 (b)), for example, as $\dot{x} = -G_x^{-1}\partial F(1)(x) - \text{div}_{S} \partial \Psi^*_x [F(2)(x)]$ where $F(1)(x)$ and $F(2)(x)$ could be different. This flexibility may contribute to the design of new algorithms for machine learning. Actually, this integrated representation is quite relevant to the filtering equations[154] in sequential inference where the first term, i.e., $-G_x^{-1}\partial F(1)(x)$, can usually be associated with the update of posterior probability by observation and the second term, $-\text{div}_{S} \partial \Psi^*_x [F(2)(x)]$ can represent the prediction by the prior information on the dynamics. Our framework may provide a unified information-geometric perspective to various information-geometric analyses and extensions of filtering, e.g., projection-filters[155], information-geometric nonlinear filtering[156], and information geometric optimization[69]. Furthermore, the generalized gradient flow can be regarded as a continuous time limit of the mirror descent where the nonlinear Legendre duality between primal and dual spaces is preserved at the limit. This fact may be employed to design new gradient-based algorithms based on the doubly dual flat structure.

IX. INFORMATION-GEOMETRIC PROPERTIES OF GENERALIZED NONEQUILIBRIUM FLOW

In this section, we consider the nonequilibrium flow defined by Eq. 59, i.e.,

$$\dot{x} = -\text{div}_{S} \partial \Psi^*_x \left( [\text{grad}_{S} \partial D_{\Phi}^X [x \parallel \tilde{x}]] + f_{NE} \right),$$

(135)

with $f_{NE} \neq 0$, and show how information geometry can be employed to analyze such dynamics. While we can obtain several properties of equilibrium flow independently of the detail of the thermodynamic function and the dissipation function, these functions should be related to obtaining nice properties for the nonequilibrium flow. We will observe that the thermodynamic function and the dissipation function of LMA kinetics actually have such a
A. Gradient-flow-like property and Lyapunov function of nonequilibrium flow

For the dynamics of the equilibrium flow (Eq. 56), the Bregman divergence $D_{\Phi}^X[x]\|\tilde{x}$ is a Lyapunov function. The Bregman divergence can still be a Lyapunov function even for the nonequilibrium flow (Eq. 59) under the following conditions:

**Lemma 5.** Suppose that, for all $x \in \mathcal{X}$, the force $f(x) = \text{grad}_S \partial_x D_{\Phi}^X[x]\|\tilde{x}$ is orthogonally decomposed as $f(x) = f_S(x) + f_A(x)$ where $f_S(x) := \text{grad}_S \partial_x D_{\Phi}^X[x]\|\tilde{x}_{CB}$ and $f_A(x) \in \mathcal{F}_x$ satisfy the pseudo-Hilbert-isosceles orthogonality $f_S(x) \perp_H f_A(x)$. Then $\frac{d}{dt} D_{\Phi}^X[x_t]\|\tilde{x}_{CB} \leq 0$ holds. In addition, $x_{CB} = \mathcal{P}^{sc}(x_0) \cap \mathcal{M}^{eq}(\tilde{x}_{CB})$ is the unique steady state of Eq. 59 with the initial state $x_0$ that attains $\frac{d}{dt} D_{\Phi}^X[x_t]\|\tilde{x}_{CB} = 0$. Thus, $x_{CB}$ is locally and asymptotically stable\[^{[81]}\].

**Proof.** We can directly verify $\frac{d}{dt} D_{\Phi}^X[x_t]\|\tilde{x}_{CB} \leq 0$ as follows:

$$\frac{d}{dt} D_{\Phi}^X[x_t]\|\tilde{x}_{CB} = \langle \dot{x}, \partial_x D_{\Phi}^X[x_t]\|\tilde{x}_{CB} \rangle = -\langle \text{div}_S j(x), \partial_x D_{\Phi}^X[x_t]\|\tilde{x}_{CB} \rangle$$

$$= -\langle j(x), \text{grad} \partial_x D_{\Phi}^X[x_t]\|\tilde{x}_{CB} \rangle$$

$$= -\langle j(x), f_S(x) \rangle = -D_{\Phi}^{x,F}[j(x)] - \tilde{f}(x) \leq 0 \quad (137)$$

where we used Eq. 119 and $\tilde{f}(x) := f_S(x) - f_A(x)$. The equality holds if and only if $f(x) = -\tilde{f}(x)$, which means that

$$f(x) = -f''(x) \iff f_S(x) = 0 \iff \text{grad} \partial_x D_{\Phi}^X[x]\|\tilde{x}_{CB} = 0 \iff x \in \mathcal{M}^{eq}(\tilde{x}_{CB}). \quad (138)$$

Because $x_t \in \mathcal{P}^{sc}(x_0)$, $x_{CB} = \mathcal{P}^{sc}(x_0) \cap \mathcal{M}^{eq}(\tilde{x}_{CB})$ holds. \[\square\]

Thus, if the pseudo-Hilbert-isosceles orthogonal decomposition exists, then the nonequilibrium flow behaves like the equilibrium gradient flow.

B. Complex-balanced state and pseudo-Hilbert-isosceles orthogonality

More specific conditions or situations under which the orthogonal decomposition in Prop. 5 exists is still an open problem. However, for CRN with LMA kinetics, the decomposition holds if a complex-balanced steady state exists.

\[^{[81]}\]To have global stability, we have to consider the boundary of $\mathcal{X}$.
Proposition 9 (Complex-balanced steady state and orthogonal decomposition for CRN with LMA kinetics\cite{77, 78, 80, 82}). Suppose that a complex balanced steady state exists, i.e., $\mathcal{M}^{CB} \neq \emptyset$ for CRN with LMA kinetics (Eq. 12). Using any $\bar{x}_{CB} \in \mathcal{M}^{CB}$, consider a decomposition of the force $f_{MA}(x)$ as $f_{MA}(x) = f_{S}(x) + f_{A}$ where $f_{S}(x) = \text{grad}_{x}D_{\Phi}[x\|\bar{x}_{CB}]$, $f_{A} = \ln K + S^{T}\ln \bar{x}_{CB}$, and $\Phi(x)$ is as in Eq. 61. Then, for the dissipation functions in Eq. 67, the pseudo-Hilbert isosceles orthogonality $f_{S}(x) \perp f_{A}$ holds for all $x \in \mathcal{X}$. In addition, $\mathcal{M}^{eq}(\bar{x}_{CB}) = \mathcal{M}^{CB}$ holds.

Proof. We can prove the orthogonality by direct computation. The orthogonality condition

$$\Psi_{x}^{*}[f_{S}(x) + f_{A}] = \Psi_{x}^{*}[f_{S}(x) - f_{A}]$$

$$\iff \left< j_{MA}^{+}(x), \left( \frac{x}{x_{CB}} \right)^{-S^{T}} - 1 \right> + \left< j_{MA}^{-}(x), \left( \frac{x}{x_{CB}} \right)^{S^{T}} - 1 \right> = 0.$$  \hspace{1cm} (139)

Consider the following equality:

$$\left< j_{MA}^{\pm}(x), \left( \frac{x}{x_{CB}} \right)^{\mp S^{T}} - 1 \right> = \sum_{e=1}^{N_{e}} k_{e}^{\mp} x_{CB}^{\pm} \left[ \left( \frac{x}{x_{CB}} \right)^{\gamma_{e}^{\pm}} - \left( \frac{x}{x_{CB}} \right)^{\gamma_{e}^{\mp}} \right],$$

where $\gamma_{e}^{\pm} := \frac{1}{k_{e}^{\pm}} b_{e}^{\pm}$. By using this, we have the following:

$$\text{Eq. 140} = \sum_{e=1}^{N_{e}} \left( k_{e}^{+} x_{CB}^{+} - k_{e}^{-} x_{CB}^{-} \right) \left[ \left( \frac{x}{x_{CB}} \right)^{\gamma_{e}^{-}} - \left( \frac{x}{x_{CB}} \right)^{\gamma_{e}^{+}} \right]$$

$$= \left< j_{MA}^{+}(\bar{x}_{CB}) - j_{MA}^{-}(\bar{x}_{CB}), \left[ \left( \frac{x}{x_{CB}} \right)^{\text{IE}^{-}} - \left( \frac{x}{x_{CB}} \right)^{\text{IE}^{+}} \right] \right>$$

$$= \left< j_{MA}(\bar{x}_{CB}), \mathbb{B}_{-}^{T} \left( \frac{x}{x_{CB}} \right)^{\text{IE}^{-}} - \mathbb{B}_{+}^{T} \left( \frac{x}{x_{CB}} \right)^{\text{IE}^{+}} \right> = \left< \mathbb{B} j_{MA}(\bar{x}_{CB}), \left( \frac{x}{x_{CB}} \right)^{\text{IE}} \right>.$$  \hspace{1cm} (142)

Thus, Eq. 139 holds for $x \in \mathcal{X}$ if $\mathbb{B} j_{MA}(\bar{x}_{CB}) = 0$ holds\footnote{The transformation of Eq. 140 here is strongly dependent on the specific functional form of $j_{MA}(x)$.}. $\mathcal{M}^{eq}(\bar{x}_{CB}) = \mathcal{M}^{CB}$ can be proved by obtaining the parametric representation of $\mathcal{M}^{CB}$ as $\mathcal{M}^{CB} = \{ x \in \mathcal{X} | \ln x - \ln \bar{x}_{CB} \in \text{Ker} S^{T} \}$ via solving $j_{MA}(x) = 0$\footnote{We skip the derivation because it is involved.}. This representation is identical to that of $\mathcal{M}^{eq}(\bar{x}_{CB})$ (Eq. 96). \hfill \Box

\footnote{We see the original derivation\cite{100} or our rephrased version\cite{83}}

[
63
]
Remark 9 (Algebraic structure of detailed balanced and complex balanced manifolds). We here mention about the underlying algebraic source of why $M_{eq}(\tilde{x}_{CB}) = M_{CB}$ holds. First, we already showed that $M_{DB} = M_{eq}(\tilde{x})$ holds generally if $M_{DB} \neq \emptyset$. Under LMA kinetics (Eq. 12), the DB condition $j_{MA}(x) = 0$ is nothing but the binomial equations because $j_{MA}(\pm x)$ is a vector of monominals of $x$. Owing to this, $M_{DB}$ becomes a toric variety. In contrast, the CB condition $\mathbb{B}j_{MA}(x_{CB}) = 0$ is a set of polynomial equations for LMA kinetics. Nonetheless, it was shown that $M_{CB}$ is binomially generated and has the same structural matrix $S^T$ as the equilibrium manifold. Because of that, they are equivalent as manifolds.

Because rLDG (Eq. 3) is a subclass of CRN where $L = I$ and thus $S = \mathbb{B}$ holds, the complex-balanced condition is always satisfied for rLDG.

Corollary 1 (rLDG is unconditionally complex-balanced[8]). All the steady states of rLDG are complex-balanced states, i.e., $M_{ST} = M_{CB}$ independently of the parameter values $k_{\pm}$ of the flux (Eq. 3) [85]. Thus, KL divergence (Eq. 63) always works as a Lyapunov function of rLDG, such as Markov jump processes.

The properties described in this corollary are well-known for MJP and are usually obtained by using the Perron-Frobenius theorem for linear operators. The framework of the generalized flow enables us to extend them to the nonlinear regime.

C. Effective flow of the nonequilibrium flow by the primal information-geometric projection

In general, the nonequilibrium force or flux has redundant degrees of freedom in terms of generating a specific vector field or trajectory $x_t$ on the vertex spaces. By using the generalized HHK projective decomposition (Thm. 1), we can carve out the effective part of the flux for the trajectory. In addition, we can obtain an effective time-dependent equilibrium flow that mimics a trajectory $\{x_t\}$ of time-independent nonequilibrium flow:

---

[84] The real variety generated by a toric ideal, i.e., a [86] More generally, if $\text{Rank}[S] = \text{Rank}[\mathbb{B}]$, CRN is un-bibinomial and prime ideal[100]. conditionally complex balanced. This condition is called the deficiency zero condition[8].

[85] Such a situation is called unconditionally complex balanced.
Lemma 6 (Effective flux and effective time-dependent equilibrium flow). Suppose that \( \mathbf{j}(\mathbf{x}) \) is the flux of a generalized flow (Eq. 43), and define the corresponding effective flux by \( \mathbf{j}_{eq}(\mathbf{x}) = \partial \Psi^*_x \left[ S^T \mathbf{u}_{eq}(\mathbf{x}) \right] \) where \( \mathbf{u}_{eq}(\mathbf{x}) := \partial \tilde{\Psi}_x \left[ -\mathbf{S} \mathbf{j}(\mathbf{x}) \right] \). Then, \( \mathbf{j}_{eq}(\mathbf{x}) \) generates the same trajectory as \( \mathbf{j}(\mathbf{x}) \) does. Furthermore, for a given trajectory \( \{ \mathbf{x}_t \} \), we can construct a time-dependent equilibrium flow \( \mathbf{j}_{eq}(t, \mathbf{x}) \) that can generate the same \( \{ \mathbf{x}_t \} \) as follows

\[
\mathbf{j}_{eq}(t, \mathbf{x}) := \partial \Psi^*_x \left[ \text{grad}_S \partial \Phi^*_{\mathbf{x}}[\mathbf{x}||\mathbf{x}_t] \right], \quad \mathbf{x}_t := \partial \Phi^*[\partial \Phi(\mathbf{x}_t) - \mathbf{u}_{eq}(\mathbf{x}_t)].
\]

Proof. From Thm. 1, \( \mathbf{j}(\mathbf{x}) \) can be decomposed as \( \mathbf{j}(\mathbf{x}) = \mathbf{j}_{eq}(\mathbf{x}) + (\mathbf{j}(\mathbf{x}) - \mathbf{j}_{eq}(\mathbf{x})) \). Because \( \mathbf{f}_{eq}(\mathbf{x}) = \partial \Psi^*_x \left[ \mathbf{j}_{eq}(\mathbf{x}) \right] \in \mathcal{P}^f(0) \), there exists \( \mathbf{u}_{eq}(\mathbf{x}) \) satisfying \( S^T \mathbf{u}_{eq}(\mathbf{x}) = \mathbf{f}_{eq}(\mathbf{x}) \). By employing the duality introduced in Thm. 2, \( \mathbf{u}_{eq}(\mathbf{x}) \) can be represented as \( \mathbf{u}_{eq}(\mathbf{x}) = \partial \tilde{\Psi}_x [\mathbf{v}(\mathbf{x})] \) where \( \mathbf{v}(\mathbf{x}) = -\mathbf{S} \mathbf{j}(\mathbf{x}) \). Because \( -\mathbf{S} \mathbf{j}_{eq}(\mathbf{x}) = \mathbf{v}(\mathbf{x}) \), \( \mathbf{j}_{eq}(\mathbf{x}) \) generates the same dynamics or vector field as \( \mathbf{j}(\mathbf{x}) \) does. By solving \( \mathbf{u}_{eq}(\mathbf{x}_t) = \partial \Phi(\mathbf{x}_t) - \partial \Phi(\mathbf{x}_t) \), we have Eq. 145. □

The effective time-dependent flow is more explicitly obtained for CRN with LMA kinetics:

Corollary 2 (Effective flow for LMA kinetics). Consider the following quantities of CRN with LMA kinetics:

- **Flux defined in Eq. 12**
  \[ \mathbf{j}_{MA}(\mathbf{x}; \mathbf{k}^\pm) \]

- **Force defined in Eq. 69**
  \[ \mathbf{f}_{MA}(\mathbf{x}; \mathbf{K}) \]

- **Thermodynamic function defined in Eq. 61**
  \[ \Phi(\mathbf{x}) \]

- **Dissipation functions defined in Eq. 67 with Eq. 69**
  \[ \Psi^*_x,\kappa[\mathbf{f}] = \Psi^*_\omega_{MA}(\mathbf{x};\kappa)[\mathbf{f}], \]

where \( \mathbf{k}^\pm = \kappa \circ \mathbf{K}^{\pm1/2} \) holds. For the trajectory \( \mathbf{x}_t \) generated by \( \mathbf{j}_{MA}(\mathbf{x}; \mathbf{k}^\pm) \), the effective time-dependent equilibrium force \( \mathbf{f}_{eq}(t, \mathbf{x}) \) can be described as \( \mathbf{f}_{MA}(\mathbf{x}; \mathbf{K}_{eq}(t)) \) where \( \mathbf{K}_{eq}(t) \) is determined by

\[
\mathbf{K}_{eq}(t) := \exp \left[ S^T (\mathbf{u}_{eq}(\mathbf{x}_t; \kappa) - \partial \Phi(\mathbf{x}_t)) \right], \quad \mathbf{u}_{eq}(\mathbf{x}_t; \kappa) := \partial \tilde{\Psi}_{x_t,\kappa} [-\mathbf{S} \mathbf{j}_{MA}(\mathbf{x}_t)]
\]

Thus, the effective time-dependent flux \( \mathbf{j}_{eq}(t, \mathbf{x}) \) is represented as \( \mathbf{j}_{eq}(t, \mathbf{x}) = \mathbf{j}_{MA}(t, \mathbf{x}; \mathbf{k}_{eq}^\pm(t)) \) where \( \mathbf{k}_{eq}^\pm(t) = \kappa \circ \mathbf{K}_{eq}^{\pm1/2}(t) \).

\[\text{[87]} \mathbf{j}_{eq}(\mathbf{x}) \text{ may not be equilibrium flux because } \mathbf{u}_{eq}(\mathbf{x}) \text{ is not necessarily represented by the gradient of a certain function } \mathcal{F}(\mathbf{x}) \text{ as } \mathbf{u}_{eq}(\mathbf{x}) = \partial \mathcal{F}(\mathbf{x}).\]
This corollary means that the effective time-dependent flux of LMA kinetics is always obtained by a time-dependent modulation of the parameter $k^{\pm}$ of LMA kinetics\footnote{While this result may not be so important mathematically, for physics and chemistry, the results means that the effective flux is physically realizable within the LMA kinetics by parameter modulation. If the effective flux is out of the LMA kinetics, its physicochemical realization becomes highly nontrivial. The same applies to rLDG.}.

D. Characterization of the nonequilibrium flow by the dual information geometric projection

The nonequilibrium flow is redundant in terms of generating a specific vector field or trajectory $\{x_t\}$. However, such redundancy is crucial to characterize the extent of nonequilibrium. One approach for the characterization is to investigate the cycle force or flux, which has been employed in the linear theory of dynamics on graphs and also in graph-theoretic approaches to nonequilibrium phenomena\cite{90, 157–160}. To extract such cyclic components, we can use $V^T = \text{curl}_V$, its adjoint $V = \text{curl}^*_V$, the associated cycle subspaces $C^2(\mathbb{H})$ and $C_2(\mathbb{H})$, and also the generalized HKK decomposition (Thm. 1).

**Definition 34 (Cycle spaces).** The cycle spaces at $x \in \mathcal{X}$ are defined as $Z_x = C_2(\mathbb{H}) = \text{Ker}[V]$ and $\mathcal{Z}_x = C^2(\mathbb{H}) = \text{Im}[V^T]$.

For a given nonequilibrium force $f(x)$, we can obtain its cycle component $\zeta = \text{curl}_V f(x) = V^T f(x) \in \mathcal{Z}_x$. $\zeta$ contains the information to categorize the force because $\mathcal{P}^{fr}(f) = \mathcal{P}^{fr}(\zeta)$ is the quotient space of force by the gradient force. For each $\zeta \in \mathcal{Z}_x$, we obtain the representative force $f^\circ(x, \zeta)$ via the following variational problem:

**Lemma 7 (Steady (zero-velocity) force as the minimizer of the dual dissipation).** For a given $\zeta \in \mathcal{Z}_x$, we define the force $f^\circ(x, \zeta)$ minimizing the dual dissipation:

$$
\begin{equation}
    f^\circ(x, \zeta) := \arg \min_{f} \Psi^*_x[f], \quad \text{s.t.} \quad \text{curl}_V f = \zeta.
\end{equation}
$$

Then, $f^\circ(x, \zeta)$ is the steady (zero-velocity) force, i.e., $j^\circ = \partial\Psi^*_x[f^\circ] \in \mathcal{P}^{vl}(0)$.

**Proof.** From Eq. 110 in Thm. 1, $f^\circ(x, \zeta) \in \mathcal{P}^{fr}(\zeta) \cap \mathcal{M}^{vl}(0)$. Thus, $j^\circ \in \mathcal{P}^{vl}(0)$. \hfill $\square$
Among various \( f \) that has the same cyclic component \( \zeta \), the force \( f^\diamondsuit(x, \zeta) \) is the one inducing no dynamics of \( x \). Because any dynamics of \( x \) can be represented by the effective flux as in Lemma 6, \( f^\diamondsuit(x, \zeta) \) can be regarded as the force being purely relevant to the cycle.

Using \( f^\diamondsuit(x, \zeta) \), we can establish the induced duality between \( Z_x \) and \( \mathfrak{J}_x \) spaces:

**Theorem 3** (Induced Hessian geometric structure on cycle spaces). On the cycle spaces, \( Z_x \) and \( \mathfrak{J}_x \), we have the Legendre conjugate dissipation functions \( \hat{\Psi}_x : Z_x \to \mathbb{R} \) and \( \hat{\Psi}^*_x : \mathfrak{J}_x \to \mathbb{R} \) induced by the dissipation functions on the edge spaces (Fig. 7 (c)).

**Proof.** For each \( \zeta \in \mathfrak{J}_x \), we can uniquely determine \( f^\diamondsuit(x, \zeta) \in \mathcal{F}_x \), \( j^\diamondsuit(x, \zeta) \in \mathcal{J}_x \), and \( z^\diamondsuit(x, \zeta) \in Z_x \) as

\[
\begin{align*}
f^\diamondsuit(x, \zeta) &:= \mathcal{P}^{fr}(\zeta) \cap \mathcal{M}^{s}_{x}(0) = \operatorname{arg} \min_{f \in \mathcal{P}^{fr}(\zeta)} \Psi_x[f], \quad (152) \\
j^\diamondsuit(x, \zeta) &:= \partial \Psi_x[f^\diamondsuit(x, \zeta)] \in \mathcal{P}^{id}(0), \quad (153) \\
z^\diamondsuit(x, \zeta) &:= (\mathcal{V})^+ j^\diamondsuit(x, \zeta), \quad (154)
\end{align*}
\]

where \((\mathcal{V})^+\) is the pseudo-inverse of \( \mathcal{V}^{[89]} \). They satisfy

\[
\zeta = \mathcal{V}^T f^\diamondsuit(x, \zeta), \quad f^\diamondsuit(x, \zeta) = \partial \Psi_x[j^\diamondsuit(x, \zeta)], \quad j^\diamondsuit(x, \zeta) = \mathcal{V} z^\diamondsuit(x, \zeta). \quad (155)
\]

Conversely, for a given \( z \in Z_x \), we have \( j^\bullet(x, u) \), \( f^\bullet(u) \), and \( \zeta^\bullet(x, u) \) as follows:

\[
\begin{align*}
\zeta^\bullet(x, z) &= \mathcal{V}^T f^\bullet(x, z), \quad f^\bullet(x, z) = \partial \Psi_x[j^\bullet(z)], \quad j^\bullet(z) = \mathcal{V} z. \quad (156)
\end{align*}
\]

Thus, for a pair of \((z, \zeta)_x\) that satisfies \( z = z^\diamondsuit(x, \zeta) \), \( \zeta = \zeta^\bullet(x, z) \), \( f^\diamondsuit(x, \zeta) = f^\bullet(x, z) \), and \( j^\diamondsuit(x, \zeta) = j^\bullet(z) \) hold. This pairing establishes a bijection between \( Z_x \) and \( \mathfrak{J}_x \). This bijection is realized by the Legendre transformations of the following induced dissipation functions on \( Z_x \) and \( \mathfrak{J}_x \):

\[
\hat{\Psi}_x(z) := \Psi_x(j^\bullet(z)), \quad \hat{\Psi}^*_x(\zeta) := \Psi^*_x(f^\diamondsuit(x, \zeta)). \quad (157)
\]

These functions are Legendre conjugate as follows:

\[
\begin{align*}
\max_{z' \in Z_x} \left[ \langle z', \zeta \rangle - \hat{\Psi}_x(z') \right] & = \max_{z' \in Z_x} \left[ \langle z', \mathcal{V}^T f \rangle - \hat{\Psi}_x(z') \right] \\
& = \max_{j' \in \mathcal{P}^{fr}(0)} \left[ \langle j', f \rangle - \Psi_x(j') \right] \\
& = \max_{j' \in \mathcal{P}^{fr}_x} \left[ \langle j', f^\Diamond(x, \zeta) \rangle - \Psi_x(j') \right] \\
& = \max_{j' \in \mathcal{P}^{fr}_x} \left[ \langle j', f^\Diamond(x, \zeta) \rangle - \Psi_x(j') \right] = \Psi^*_x(f^\diamondsuit(x, \zeta)) = \hat{\Psi}^*_x(\zeta), \quad (158)
\end{align*}
\]

[89] Because \( \mathcal{V} : Z_x \to \mathfrak{J}_x \), \( j^\diamondsuit(x, \zeta) \in \mathcal{P}^{sc}(0) = \operatorname{Im}[\mathcal{V}] \) and \( \operatorname{Ker}[\mathcal{V}] = \{0\} \), \((\mathcal{V})^+\) is uniquely determined.
Thus, the effective cycle flux $j^\circ(x, \zeta) = 0$ because $j^\circ \in \mathcal{P}^{sc}(0) = \text{Im} V$ and $f - f^\circ(x, \zeta) \in \mathcal{P}^{fr}(0) = \text{Ker} V^T$. The inverse is also shown:

$$\max_{\zeta \in \mathcal{K}_x} \left[ \langle z, \zeta \rangle - \hat{\Psi}_x(\zeta) \right] = \max_{\zeta \in \mathcal{K}_x} \left[ \langle z, V^T f^\circ(x, \zeta) \rangle - \hat{\Psi}_x^*(f^\circ(x, \zeta)) \right]$$

$$= \max_{f^\circ \in \mathcal{P}^{sc}_x(0)} \left[ \langle z, f^\circ \rangle - \hat{\Psi}_x^*(f^\circ) \right] = \max_{f^\circ \in \mathcal{P}^{sc}_x(0)} \left[ \langle j^\bullet(z), f^\circ \rangle - \hat{\Psi}_x^*(f^\circ) \right]$$

$$= \hat{\Psi}_x(j^\bullet(z)) = \hat{\Psi}_x(z)$$

The pair $(z, \zeta)_x$ is Legendre dual with respect to these functions:

$$\partial_{\zeta} \hat{\Psi}_x^*(\zeta) = \left[ \frac{\partial f^\circ(x, \zeta)}{\partial \zeta} \right]^T \left[ \frac{\partial \Psi_x^*(f)}{\partial f} \right]_{f = f^\circ(x, \zeta)} = \left[ \frac{\partial f^\circ(x, \zeta)}{\partial \zeta} \right]^T f^\circ(x, \zeta) \quad (158)$$

$$\partial_z \hat{\Psi}_x(z) = \left[ \frac{\partial j^\bullet(z)}{\partial z} \right]^T \left[ \frac{\partial \Psi_x(j)}{\partial j} \right]_{j = j^\bullet(z)} = \left[ \frac{\partial j^\bullet(z)}{\partial z} \right]^T f^\bullet(x, z) = V^T f^\bullet(x, z) = \zeta, \quad (160)$$

where we used $\left[ \frac{\partial f^\circ(x, \zeta)}{\partial \zeta} \right]^T \zeta = I$ from $\frac{\partial}{\partial \zeta} [\zeta - V^T f^\circ(x, \zeta)] = I - V^T \frac{\partial f^\circ(x, \zeta)}{\partial \zeta} = 0$ and $\frac{\partial j^\bullet(x, z)}{\partial z} = \zeta$. They are dissipation functions: strict convexity and 1-coercivity follow from those of the original dissipation functions. Also, we have

$$(\text{Symmetry}) \quad \hat{\Psi}_x(-z) = \Psi_x(j^\bullet(-z)) = \Psi_x(-j^\bullet(z)) = \hat{\Psi}_x(z) \quad (161)$$

$$(\text{Bounded by 0 at 0}) \quad \hat{\Psi}_x(z = 0) = \Psi_x(j^\bullet(0)) = \Psi_x(0) = 0. \quad (162)$$

For a given force $f(x)$ of generalized flow (Eq. 43), $f_{st}(x) = f^\circ(x, V^T f(x))$ works as the effective cycle force in each $x \in \mathcal{X}$. Similarly to Cor. 2, we obtain the effective cycle force and the flux for LMA kinetics by parametric modulation:

**Corollary 3** (Effective cycle force and flux for LMA kinetics). Consider CRN with LMA kinetics as in Cor. 2. For each $x \in \mathcal{X}$, the effective cycle force $f_{st}(x)$ associated with $j_{MA}(x; k^\pm)$ can be described as $f_{st}(x) = f_{MA}(x; K_{st}(x))$ where $K_{st}(x)$ is determined by

$$K_{st}(x) := \exp \left[ f^\circ(x; V^T f_{MA}(x; K)) - S^T \partial \Phi(x) \right]. \quad (163)$$

Thus, the effective cycle flux $j_{st}(x)$ is represented as $j_{st}(x) = j_{MA}(x; k_{st}^\pm(x))$ where $k_{st}^\pm(x) = \kappa \circ K_{st}^{\pm 1/2}(x)$. 

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In modern nonequilibrium thermodynamics, the effective flux and force, $j_{st}(x)$ and $f_{st}(x)$, have been associated with the housekeeping EPR $\dot{\Sigma}^{hk} := \langle j_{st}(x), f_{st}(x) \rangle$, which quantifies the part of dissipation in the nonequilibrium dynamics, which stays non-zero if the trajectory is kept at $x$ or even at the real steady state $x_{st} \in \mathcal{M}^{st}$. The remaining part $\dot{\Sigma}^{ex} := \dot{\Sigma} - \dot{\Sigma}^{hk}$ is also called excess EPR, which is nonzero transiently and becomes zero at the steady state. Thus, the dually flat structure on the edge space and the HHK decomposition provide a way to dissect the steady and transient aspect in the nonequilibrium flow.

X. SUMMARY AND DISCUSSION

In this work, we have clarified that the doubly dual flat structure of the vertex and edge spaces on graphs and hypergraphs provides the information-geometric basis for the dynamics on graphs and hypergraphs as equilibrium and nonequilibrium flows. Two notions of orthogonality, pseudo-Hilbert isosceles orthogonality and information-geometric orthogonality, have been introduced and shown to dissect the equilibrium and nonequilibrium aspects of the dynamics as the induced structures on the tangent and cotangent spaces and the cycle spaces, the former of which is a generalization of the Otto structure. This structure naturally connects the topological information of underlying discrete manifolds, i.e., graphs and hypergraphs, with the dynamics on them and thus endows more flexibility and representation power to the information-geometric modeling of dynamics. Furthermore, the generalized equilibrium and nonequilibrium flow, as well as the generalized flow, accommodate a sufficiently wide range of models, which include the reversible Markov jump processes on finite graphs and CRN with LMA kinetics (a class of PDS). These results could substantially extend the applicability of information geometry to dynamical problems and open up a new connection between information geometry and homological algebra.

[90] It should be noted that various definitions of housekeeping and excess EPRs have been proposed in nonequilibrium thermodynamics. The definition here is just one of them. It is an open problem how to define the notion of effective entropy for nonequilibrium dynamics.
A. Extension of other relations involving information measures

While we demonstrated that the generalized flow and the two dual flat structures can generalize several results known for FPE and diffusion processes, we still have potentially relevant results and problems that could be explained and extended in our framework. For example, for FPE and diffusion processes, the Fisher information number $I_F$ was extended to the relative Fisher information (also known as Hyvärinen divergence[122, 146]). The relative Fisher information of two trajectories $p_i^{(1)}(r)$ and $p_i^{(2)}(r)$ are known to satisfy information-theoretic relations such as the De Brujin identity[53] and its extensions[55, 61]. In addition, the logarithmic Sobolev inequality also constitutes a relationship between the Fisher information number and the KL divergence (or Shannon information)[62, 63]. It would be an important future problem to integrate these results into the doubly dual flat structure.

Moreover, several relations potentially being related to De Giorgi’s formulation (Eq. 50) have been known for mutual information in filtering and control theories. For example, Guo, Shamai, and Verdu found a relation between mutual information and the minimum mean square error (MMSE) in Gaussian channels [161]. Relations similar to these have also been reported by Mayer-Wolf and Zakai[162, 163]. Our framework may offer a unified perspective behind these different types of relation involving information measures.

B. Extensions of the doubly dual flat structure

There is also room for extensions of the doubly dual flat structure. While we consider only strictly convex thermodynamic functions and dissipation functions, strict convexity is not necessarily required, at least for defining the generalized flow and the equilibrium and nonequilibrium flows[91]. Actually, in terms of thermodynamics, the thermodynamic function can be non-strictly convex when a phase transition of the system occurs [118]. The loss of bijectivity via the loss of the strict convexity can happen in complicated and degenerate statistical models[164]. Techniques from algebraic geometry could be employed to address such situations[165].

[91] The strict convexity of the dissipation functions is assumed to work on the projections in the edge spaces where the bijection between $J_x$ and $F_x$ are important. Injectivity of $\partial \Psi^*_x$ and $\partial \Phi$ is sufficient to define the generalized flow and equilibrium and nonequilibrium flow.
Moreover, the structure introduced for reversible LDG and CRN may be extended to irreversible cases, where some edges have only either forward or reverse jumps or reactions. For this purpose, we may take advantage of several results about the CB states obtained in CRN theory [8] where the reversibility is not necessarily assumed and those in stochastic thermodynamics for absolute irreversible processes [166].

While the nonequilibrium flow is general enough to cover at least all reversible CRN with LMA kinetics, the classes of nonlinear dynamics other than CRN or PDS are much wider than that in general. To further extend the range of models that can be covered, GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) would be a good candidate [167]. GENERIC is a theoretical framework to integrate dissipative dynamics (gradient flow dynamics) and conservative dynamics (Hamiltonian dynamics). The extension of the generalized flow to GENERIC has already been attempted, but is still ongoing [76, 78]. The information geometry could offer new insights and techniques to achieve this mission.

C. Homological algebraic and differential geometric formulations

From the viewpoint of the standard homological algebra, the doubly dual flat structure that we introduced is an extension of chain and cochain complexes with inner product structure to those with the Legendre dual structure. Because the homological algebra used here is an abstraction of the differential form, the doubly dual flat structure can also be viewed as an extension of the differential form and might be called dually flat form. It is an interesting mission to characterize this stricture under a more rigorous mathematical formulation and to investigate if the Legendre duality can be consistently introduced for chains and cochains higher than those of the edge space. From the viewpoint of differential geometry, the dual flat structure is characterized independently of the specific coordinate by the Hessian manifold[147]. While we stick to the standard basis of the graph or hypergraph on which the convex thermodynamic function is defined, we can formulate it by using Hessian geometry more generally. It would be an important future work to clarify how the doubly dual flat structure is formulated from a differential geometric perspective.
D. Consistency and Persistence

Finally, we mention the problem of consistency and persistence. In this work, we presume that the flux $j(x)$ is consistent with $H$ and that the trajectory is persistent. The explicit conditions when they are satisfied are still elusive. Actually, the sufficient condition for consistency is intricate, even for the separable cases. For an illustrative example, suppose that the $i$th molecule is involved in the $e$th reaction of a CRN with LMA kinetics. For $x_i \to 0$, $j_e(x) \to 0$ holds. However, their Legendre duals diverge as $y_i \to -\infty$ and $f_e(x) \to -\infty$. $j_e(x)$ goes to 0 because $\omega_e(x) \to 0$ holds. This example suggests that we have to consider a certain limit of relevant quantities to appropriately address the consistency condition.

The persistence of the nonequilibrium flow would be a much harder problem. While the persistence was proven for CB CRN with LMA kinetics using techniques from algebraic geometry[113], its connection to information geometry has yet to be clarified. Moreover, from the information-geometric viewpoint, the loss of persistence means the change in the support of probability or positive density, which is effectively accompanied by the change in the topology of the underlying graph or hypergraph. To resolve the problem, we may need a deeper understanding of the interrelationship among dynamics, information-geometric structure, and the underlying topology.

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Appendix A: Symbols, Notations, and Abbreviations
| Symbol | Description                                                                 | Section/Definition |
|--------|-------------------------------------------------------------------------------|--------------------|
| $G$, $G_{k^+}$ | finite graph and edge-weighted finite graph.                                 | Def. 1             |
| $v$, $e$ | vertex and edges of graph $G$.                                               | Def. 1             |
| $\mathbb{B}$ | incidence matrix                                                               | Def. 1             |
| $H$, $H_{k^+}$ | Reversible CRN hypergraph and edge-weighted finite graph.                    | Def. 4             |
| $X$, $\hat{X}$, $e$ | vertex, hypervertex, and hyperedges of CRN hypergraph $H$.                   | Def. 4             |
| $S$ | Hypergraph incidence matrix.                                                  | Def. 4             |
| $\mathbb{L}$ | Hypervertex matrix                                                            | Def. 4             |
| $C_p(G)$, $C^p(G)$ | $p$-chain and $p$-cochain of graph with field $\mathbb{R}$                   | Sec. III A         |
| $C_p(H)$, $C^p(H)$ | $p$-chain and $p$-cochain of hypergraph with field $\mathbb{R}$              | Def. 9             |
| $\delta_p$, $\delta^p$ | $p$-discrete differentials                                                      | Sec. III A, Def. 9 |
| $\text{grad}_S := \delta^0 = S^T$ | Discrete gradient                                                             | Def. 10            |
| $\text{div}_S = \text{grad}^*_S := \delta_1 = S$ | Discrete divergence (adjoint of discrete gradient)                           | Def. 10            |
| $\text{curl}_V := \delta^1 = \nabla^T$ | Discrete curl                                                                | Def. 10            |
| $\text{curl}^*_V := \delta_2 = \nabla$ | Adjoint of discrete curl                                                      | Def. 10            |

TABLE I. List of symbols and notations related to graph, hypergraph and homological algebra.
| Symbol | Definition/Description |
|--------|-----------------------|
| $X, Y$ | Primal and dual vertex spaces (density and potential spaces) |
| $x$    | The density defined on vertices of graph or hypergraph |
| $y$    | The potential field defined on vertices of graph or hypergraph |
| $J_x, F_x$ | Primal and dual edge spaces |
| $j^+, j^-$ | The forward and reverse oneway fluxes of graph or hypergraph |
| $j$    | The total flux on edges of graph or hypergraph |
| $f$    | The force on edges of graph or phyergraph |
| $j^e_{MA}, j^e_{eMA}$ | Oneway fluxes of the normal and extended LMA kinetics. |
| $j_{FP}$ | Flux of the FPE |
| $f_{NE}$ | nonequilibrium force |
| $f_{MA}(x:K), \omega_{MA}(x:K)$ | Force and frenetic activity of LMA kinetics |
| $\mathcal{M}^{ST}$ | Steady state manifold |
| $\mathcal{M}^{CB}$ | Complex-balanced manifold |
| $\mathcal{M}^{DB}$ | Detailed-balanced manifold |
| $L_\theta$ | Weighted asymmetric graph Laplacian |

| Table II. List of symbols and notations related to the dynamics on graph and hypergraph. |
| Symbol | Description | Reference |
|--------|-------------|-----------|
| $\Phi, \Phi^*$ | Primal and dual thermodynamic functions | Def. 12, Def. 13 |
| $D_{\Phi}^X[x||x'], D_{\Phi'}^Y[y'||y]$ | Bregman divergences on vertex spaces | Def. 14 |
| $T_x\mathcal{X}, T_x^*\mathcal{X}$ | Tangent and cotangent spaces of $\mathcal{X}$ | Def. 15 |
| $T_y\mathcal{Y}, T_y^*\mathcal{Y}$ | Tangent and cotangent spaces of $\mathcal{Y}$ | Def. 15 |
| $G_x, G_y^*$ | Hessian matrices on vertex spaces | Def. 15 |
| $\Psi_x, \Psi^*_x$ | Primal and dual dissipation functions | Def. 18 |
| $D_{x^T}[j; f']$ | Bregman divergence on the edge space | Eq. 39 |
| $G_{x,j}, G^*_{x,f}$ | Hessian matrices on the edge space | Eq. 40 |
| $\tilde{\Psi}_x(x), \tilde{\Psi}^*_x(x)$ | Quadratic dissipation function | Eq. 41 |
| $\mathcal{P}^{sc}(x_0)$ | Stoichiometric subspace | Def. 26 |
| $\mathcal{P}^{eq}(\tilde{y})$ | Equilibrium subspace | Def. 27 |
| $\mathcal{P}^{vl}(\hat{j})$ | Iso-velocity subspace | Def. 28 |
| $\mathcal{P}^{fr}(f')$ | Iso-force subspace | Def. 29 |
| $\mathcal{M}^{sc}(y_0), \mathcal{M}^{eq}(\tilde{x})$ | Stoichiometric and equilibrium manifolds | Def. 30 |
| $\mathcal{M}^{vl}(f), \mathcal{M}^{fr}_x(j')$ | Iso-velocity and Iso-force manifolds | Def. 31 |
| $C^{\Psi}_x(c), C^{\Psi^*_x}(c)$ | Primal central affine manifolds | Def. 32 |
| $\mathcal{M}^{\Psi}_x(c), \mathcal{M}^{\Psi^*_x}(c)$ | Dual central affine manifolds | Def. 32 |
| $\perp_H$ | Pseudo-Hilbert-isosceles orthogonality | Def. 33 |
| $\tilde{T}_x\mathcal{X}, \tilde{T}_x^*\mathcal{X}$ | Induced tangent and cotangent spaces of $\mathcal{X}$ | Thm. 2 |
| $\tilde{\Psi}_x(v), \tilde{\Psi}^*_x(u)$ | Induced dissipation functions on tangent and cotangent spaces | Eq. 126 |
| $\mathcal{Z}_x, \mathcal{Z}_x^*$ | Cycle spaces | Def. 34 |
| $\tilde{\Psi}_x(z), \tilde{\Psi}^*_x(\zeta)$ | Induced dissipation functions on cycle spaces | Eq. 157 |

TABLE III. List of symbols and notations related to the information-geometric structure.
| CRN     | Chemical reaction network |
|---------|---------------------------|
| LMA     | Law of mass action        |
| (r)MJP  | (Reversible) Markov jump process |
| (r)LDG  | (Reversible) linear dynamics on graph |
| PDS     | Polynomial dynamical systems |
| CB      | complex-balanced          |
| DB      | detail-balanced           |

**TABLE IV.** List of abbreviations.