Algebraic Theory of Biological Organization

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Algebraic Theory of Biological Organization
生物学的組織化の代数的理論

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To my parents, grandmother and
Akiko Nishio

Contents

Chapter 1

Introduction

The famous book "What is Life?" by Erwin Schrödinger written over sixty years ago shed light on how orders in biological systems are possible from both macroscopic and microscopic points of view [97]. His macroscopic explanation simply appealed to the "$\sqrt{N}$ law" of statistical theory. That is, the order of the relative error $\sqrt{N}/N = 1/\sqrt{N}$ goes to zero as the number N of molecules becomes larger. Thus biological systems can behave faithfully in indefinite environments. This is so-called "order-from-disorder". On the other hand, his microscopic explanation was inspired by the stability resulting from discrete nature of quantum theory. Considering permanence and mutation of hereditary materials, he predicted that genetic information might be stored as molecules with aperiodic crystal structure before the discovery of the double helix structure of DNA by Watson and Crick. In contrast to "order-from-disorder" in macroscopic regime, he proposed "order-from-order" as a principle of microscopic regime in biological systems.

The principle of "order-from-order" may immediately remind us of biological systems as clockwork devices. However, any clockwork includes a principle beyond physical laws, that is, organization as a machine [78]. Any clock can in principle malfunction based on physical laws, whereas it is nonsense to say that a physical law malfunctions. What is broken in malfunction of a clock is the organization of the clock. Thus although Schrödinger tried to explain life from physical point of view, his "order-from-order" gives rise to the problem of organization [37, 38], which is a main theme of this thesis.

von Bertalanffy's general system theory is an earlier attempt to address organization of biological systems [10]. The father of modern biophysics, Nicolas Rashevsky also felt a need for general principles of biological organization [82]. Robert Rosen, who had been a student of Rashevsky, proposed a mathematical theory of biological organization in late-fifties [83, 84, 85]. Rosen's theory is based on category theory [52], which is a new mathematics developed in past 60 years. The central ingredients in category theory are relations between objects (called morphisms) rather than objects themselves, which might be significant when one addresses organization of biological systems. Category theory is a basic tool of this thesis and elementary parts of it will be used freely. Knowledge of category theory needed for reading this thesis may be found in elementary textbooks [41, 77].

Rosen did not focus on material foundations of biological systems but forms or processes of them. He tried to clarify organization of biological systems from functional point of view [91]. Here let us review his theory briefly. A recent review can be found in [44]. Let A be a set of substrates and B be a set of products. A metabolism is simply a function $f : A \to B$. The set of all possible metabolisms are denoted by $\mathrm{Hom}(A, B)$. However, since material foundations of metabolisms are protein enzymes, they have finite duration of life. Hence there must be a function that repairs metabolisms in order a cell to be alive. It is denoted by a function $\Phi : B \to \mathrm{Hom}(A, B)$. Again, material foundations of repair functions are also protein enzymes, which have finite lifetime. Thus a function of repair of repair, which is called replication by Rosen, is required. This is a function $\beta : \mathrm{Hom}(A, B) \to \mathrm{Hom}(B, \mathrm{Hom}(A, B))$. Immediately this argument can fall into infinite regress. However, biological systems indeed exist with these functional components, the infinite hierarchy must be terminated at some finite level. As a solution, Rosen proposed an isomorphism as a sufficient condition:

$$\mathrm{Hom}(A, B) \cong \mathrm{Hom}(B, \mathrm{Hom}(A, B)).$$

In his later book [92], he concluded that such an isomorphism must be constructed by an uncomputable function, which differentiates living organisms from mechanisms corresponding to computable functions. Although the authenticity of this claim is problematic [15] (see also [48]), Rosen's theory might be a first one that provides a minimal abstract model of biological organization.

In chapter 2, we re-examine the theoretical biology of Rosen. However, we will not follow the construction of Rosen reviewed here. Instead, we focus on his functional point of view itself and clarify it by category theory. We consider network representation of biological systems and work in the category of directed graphs. In functional point of view, any material represented as a node of a network is considered as a collection of its functions in the network. This operation of "decomposition into functions" can be formalized as a functor on the category of directed graphs. We can also consider the reverse operation, which we will call "gluing functions" as a functor. However, these two operations are not in general reverse of each other in mathematical sense. We will show that this displacement from true reverse provides non-trivial structures of networks which seems to be significant from biological point of view.

Speaking of theory of biological organization, we cannot forget theory of autopoiesis [62, 110, 111]. Autopoiesis is literally means "self-creation". It is defined as [110]

> a unity by a network of productions of components which (i) participate recursively in the same network of productions of components which produced these components, and (ii) realize the network of productions as a unity in the space in which the components exist.

Some computational models have been proposed considering autopoiesis [121, 70]. There are also theoretical considerations on autopoiesis in terms of category theory [68, 100]. A similar idea but with further considerations about chemical realization has been proposed [21, 22]. Recently some researchers have been attempted to realize autopoiesis as chemical systems [6, 49, 122]. Autopoiesis is a theory about characterization of the nature of biological organization [49]. However, it is not a theory about how such biological organization can be possible.

Recently, some attentions have been paid for category theory in quantum gravity (for example, [32, 54, 55, 118]). Among them, Elias Zafiris suggested that the same category or topos theoretical apparatus can be useful for complex systems research [119, 120]. Than and Tsujishita [104] used a similar tool to model process of gluing periodic observers on a dynamical system. In these works, the notion of sheaf plays a significant role. Sheaf is a well-known notion to treat parts-whole problems in mathematics [53]. Parts-whole problem would be central for biological organization since organization entails wholeness of itself. The condition of sheaf guarantees a one-to-one correspondence between locally coherent parts and wholes. In order to connect parts and wholes, a medium to do so is necessary. Mathematicians introduce the notion of topology for this aim. Moreover, a suitable topology should be defined for each parts-whole problem. In the former half of chapter 3, we will introduce a suitable topology in order to address wholeness of local structures in biological networks. However, the notion of sheaf and topology seems to be too "neat" and restricted to argue parts-whole problems in biological organization. This is the main issue of the latter half of chapter 3 and chapter 4 and 5.

In the latter half of chapter 3, we focus on information processing networks of biological systems. There are characteristic local patterns so-called network motifs common with information processing networks such as gene transcription regulation networks or neuronal networks [65]. We will argue the relationship between network motifs and information processing as a parts-whole problem. The crucial point is that each network motif is a local pattern in a whole network on one hand, the motif itself is a whole which entails a biological function, in our case, information processing.

The notion of information has several aspects. As widely known, Shannon's information theory [98] only considers the syntactic aspect of information. Both semantics and pragmatics are ignored in Shannon's theory. Probably this ignorance would enable Shannon's theory to be mathematically rigorous, however, in biology, both semantics and pragmatics may be essential aspects of information [11, 30]. Semantics is the theory about the relationships between symbols and their referents. On the other hand, pragmatics is the theory about the relationships between symbols and their users. Obviously, semantics and pragmatics are significant in communications between higher animals. Probably they might be also significant in molecular communications in a cell since living organisms are dependent on transcription and translation processes on DNA and RNA, which are indeed symbolic. Allosteric nature of bio-molecules, which can in principle associate two arbitrary biochemical processes, might also allow a broader symbolic process in a cell [67].

In Shannon's theory, information is defined as reduction of uncertainty on the presupposition that probability of occurrence of each symbol can be preassigned. An external observer that can grasp a whole situation is assumed implicitly. However, there are several definitions not dependent on such an external observer. These pay attention to semantic or pragmatic aspects of information. Gregory Bateson gave a semiotic definition of information: information is "a difference that makes a difference" [8]. Such a cascade of difference seems to be essential to biological organization since living organisms make distinctions into their environments in order to survive and in turn such distinctions in their environments affect the behaviors of them. Note that the notion of difference is effective only if a receiver of information is considered. A receiver of information is explicitly considered in the definition of pragmatic information, which is defined as an impact on receiver's structure [23]. Receiver's point of view is also relevant to consider biological functions [64]. Some authors consider information as constraints or boundary conditions for dynamics of a system [38, 72]. This view of information might be related to the hierarchical nature of biological organization [16, 71, 93, 94]. Imagine the hierarchy of human body, cells, tissues, organs and individuals. Each lower level provides constituents for a contiguous upper level on one hand, the upper level constrains the dynamics of lower level on the other hand. The distribution of lower level constituents is not determined in itself. The distribution of lower level constituents constrained by the contiguous upper level in turn has functional relevance to the upper level, for example, the arrangement of organs is crucial to the behavior of an individual.

Although information is related to many issues on biological organization, we only treat a formal aspect of it in this thesis. The structure of information processing at least consists of three constituents, sending, transforming and receiving information. This is formally represented by a directed graph with two distinct nodes and a single arrow between the two nodes. In the latter half of chapter 3, we will present how to internalize this information processing structure into nodes. We will show that such an internal structure of nodes can lead to specific local patterns of networks. Chapter 4, which is the most mathematical in this thesis, is devoted to generalizations of the result of chapter 3.

In chapter 5 and 6 we focus on change in biological organization. We here also consider network representation of biological organization. Speaking of change in biological organization, one should be careful about the distinction between evolution and development. According to Stnanley Salthe [94], evolution is "the irreversible accumulation of historical information". On the other hand, development is "predictable irreversible change". Both changes are considered to be irreversible, however, evolution is dependent on historical contingency. We should also be sensitive to the notion of information when we consider evolution [63]. Thus if evolution is considered from broader perspective than that of neo-Darwinian, it seems to be far beyond our formal treatment of biological organization at present. Hence we only treat the developmental aspect of biological organization, in particular, development of ecological networks. This seems to be too restricted, however, we do not think so since we can adopt the point of view "organisms as superecosystems" based on the fact that living organisms consist of enormously complicated material and energy flow networks [18, 108].

When some change occur in biological organization, one might notice complementarities between different disciplines such as between symbols and matters [73, 74] or between discrete and continuous [42]. The notion of robustness, which has at least two versions, one is persistence of a function with structural change and the other is switching between multiple functions with a persistent structure, is also relevant here [33]. More suitable notion for development of biological organization might be the complementarity between adaptation and adaptability [16, 109]. Adaptation mainly concerns the efficiency of a behavior of a system to a specific environment on one hand, adaptability is an ability to cope with unknown environments, which may be related to redundancy of the system, on the other hand. As a system develops, its organization may become more sophisticated and efficient whereas its redundancy decreases, which makes the system vulnerable to external perturbations. Development of a system show a specific pattern of immature, mature and senescence [94, 108]. The stage of senescence is also significant in terms of the balance between adaptation and adaptability, however, we only consider the first two stage of development in chapter 5 and 6.

The book "Ecology, the Ascendent Perspective" written by Robert Ulanowicz provides a fascinating perspective on development of biological organization [108]. This book consists of criticisms to the mechanistic view of the nature. There would be four points. First he defends the existence of ontological indeterminacy. Indeterminacy is here not considered as a result of limitations of human knowledge on the nature but is considered as intrinsic to the nature. This is an objection to the deterministic and closed nature of the mechanistic view. Second he proposes autocatalysis at the ecosystem level. Usually autocatalysis is considered as a feature of chemical reactions, however, here it is considered in broader sense. This is a critique to the atomistic nature of the mechanistic view. Third he shows the existence of "window of vitality" between the unstable region and the frozen region. All ecosystems' data he prepared fall into the "window of vitality" region. The "edge of chaos" view on life is criticized as an artifact resulting from the mechanistic view.

The fourth point is the most relevant to this thesis. This includes his autocriticism. About thirty years ago, he proposed a macroscopic index of ecosystem development, which is called ascendency [105]. Ascendency was first defined as an objective function which is to be maximized through ecosystem development. However, he later re-defined ascendency as an orientating function which only assigns the directions to which ecosystems tend to develop [108]. The assumption of macroscopic objective functions to be optimized through ecosystem development is based on the same sprit as the variational principles in classical mechanics and thermodynamics. Apparently, the notions of objective and biological organization seem to have good chemistry. However, in order an objective function to work actually, one must know all boundary conditions under which the optimization is performed. In reality, any participant in an ecosystem would act based on its local situation. Hence it takes a finite duration to propagate the effect of an action of a participant through the whole system. Thus Ulanowicz referred to only the direction of development and its tendency in the new version of ascendency hypothesis. We will provide a further discussion on this point in chapter 6.

The idea of orientating function naturally leads us to the internal perspective on biological organization [27, 56]. In short, the internalism considers how to bridge a gap between two modes, such as descriptions in the third person and in the first person, or in the present form and in the present progressive form. This is also related to the problem of rule following paradox in linguistic philosophy [25, 26, 40, 116]. We will see in chapter 5 and 6 that the notions from the internalism are useful when we try to describe changes in biological organization in our algebraic way.

One strategy to the problem of the internalism is to consider a consistency between two modes [27]. In chapter 5, we consider a negotiation process toward a consistency between inter-level process and intra-level process when describing the development of trophic hierarchy. If an inconsistency between the two processes in a system occurs then it should be eliminated in order the system to survive. If such an elimination process of an inconsistency is only performed from "enfant's eyes" then the elimination process itself could generate a new inconsistency to be resolved in a successive negotiation. We adopt such a reasoning to describe the development of trophic hierarchy in chapter 5.

The other strategy of the internalism is the emphasis on the consumer's role in energy flows [57, 59, 60] or information processing [58]. If several agents compete against each other to a single source of energy then the one who has the fastest consumption rate wins [59]. On the other hand, the energy supplier limits the total amount of energy available to the consumers. When we consider energy or material flow balancing process in biological networks [76], both suppliers and consumers of energy or material take part in how flows are regulated [57]. The present progressive form "balancing" is important. Balancing process should be distinguished from the balance between incoming flows and outgoing flows at each node. Each node in a flow network joins the network as a consumer to upstream nodes and as a supplier to downstream nodes. In turn, each flow in the network is subject to regulations by both a consumer from its downstream and a supplier from its upstream. Therefore a globally coherent mechanism of flow regulation is necessary in order to accomplish the balance at every node in a flow network. However, in reality, such a regulation would be impossible since any material interaction takes a finite duration limited by the speed of right [56]. Thus flow regulations should be considered in a local manner. If flow regulations are local then the balancing process toward a balance may generate a new imbalance to be eliminated in a successive flow regulations. In chapter 6 we will show that such balancing process can result in a self-organization of flow networks.

Throughout this thesis, we focus on the relations between relations in biological networks and how relations between relations materialize as specific patterns of biological networks. These mutually complement way of thinking are described in an algebraic way. The following first three chapters (2,3 and 4) describe the relations between relations and their materializations by purely algebraic language. In the last two chapters (5 and 6), in addition to the algebraic description of biological organization, we introduce the notions from the internalism such as consistency between two modes (chapter 5) and balancing process (chapter 6) in order to describe changes in biological organization. These chapters might seem to be rather ad hoc than the first three chapters. However, our aim in these chapters is not to provide the systematic description of changes in biological organization, but to demonstrate the usefulness of the internalism when we describe changes in biological organization.

Chapter 2

Duality between Decomposition and Gluing: A Theoretical Biology via Adjoint Functors

Two ideas in theoretical biology, “decomposition into functions” and “gluing functions”, are formalized as endofunctors on the category of directed graphs. We prove that they constitute an adjunction. The invariant structures of the adjunction are obtained. They imply two biologically significant conditions: the existence of cycles in finite graphs and anticipatory diagrams.

2.1 Introduction

The use of category theory [52] in theoretical biology dates from Robert Rosen’s pioneering works in the late 1950s [83, 84, 85]. Describing biological systems using category theory, he analyzes their properties in terms of optimality principles [85], sequential machines [86, 87, 88], category theory itself and so on. Rosen [89] gives a summary. We believe that his use of category theory is very effective. However, those who are familiar with category theory may question the fact that there is no direct use of adjoint functors in his work. Although adjoint functors are central to category theory, they do not appear explicitly in Rosen’s works. Baianu et al. [7] consider an adjunction related to the category of metabolism-repair systems. However, it appears to be an addition to Rosen’s work. Louie [46] refers to Galois theory, which is a special case of adjunctions, in relation to the categorical analysis of dynamical system theory. The Galois connection is used in wider context than that considered by Rosen.

One of the motivations of this chapter is to provide an intrinsic link between Rosen’s ideas and adjoint functors. However, we do not deal directly with

Rosen's works. In particular, we do not consider its computational aspects [47]. Instead, we consider the idea behind Rosen's work and formalize it in the category of directed graphs. We will show that Rosen's idea is one half of an adjunction. After constructing the adjunction, we find the invariant structures of the adjunction which turn out to have significant consequences for theoretical biology. They imply the existence of a cycle and conditions for anticipation.

Formally a biological system is considered to have a circular organization [44]. If a biological system is represented by a finite directed graph then the existence of a cycle indicates it has a circular organization. On the other hand, the existence of cycles in finite directed graphs is a weaker result than the condition for closure to efficient cause in metabolism-repair systems [92]. However, we can provide a more general framework in which an alternative logical route to these topics can be introduced by focusing on the adjunction that is established in this chapter.

Anticipation is another important issue in theoretical biology because it seems that anticipation is intrinsic to biological systems in relation to learning, adaptation, evolution and so on [90]. This subject has a broad scope; however, we restrict ourselves here to treating only its formal aspects.

Natural systems are usually expressed as dynamical systems that contain the temporal dimension explicitly. At first glance category theory seems to be incompatible with the temporal dimension. For example, a composite arrow in a category must exist before the composition. If one attempts to include the temporal dimension in a category, one has to consider the dynamical change of the category [19]. Such an approach regards a category as the structural pattern of a concrete system. However, this is not the only way to view a category. One can view a category as an analytical tool for investigating the common properties of certain objects. Here we take this latter point of view. In particular, an adjunction that is independent of the temporal dimension is the primary tool in the following discussion. Analysis in terms of an adjunction can be applicable to any temporally changing object as long as the object belongs to the category on which the adjunction holds.

The organization of this chapter is as follows. In section 2 we review two ideas in theoretical biology: "decomposition into functions" and "gluing functions". In sections 3 and 4 we formalize these ideas as functors on the category of directed graphs. In section 5 adjunctions are derived from these functors and their invariant structures are obtained. In section 6 we discuss the invariant structures in relation to the existence of a cycle and anticipation. In section seven we give a summary and outlook. In the appendix we provide a slightly different formalization of "decomposition into functions" and "gluing functions".

2.2 Ideas in Theoretical Biology

In the framework of Rosen's theoretical biology, an object in a system is defined by its functions. The units of a system are the functions of its constituent objects. This idea of "decomposition into functions" is the idea behind

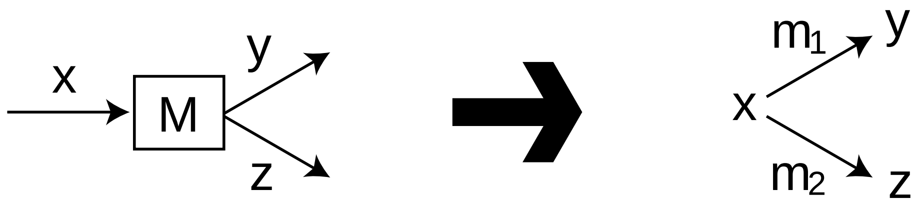

Figure 2.1: The idea in Rosen's abstract block diagrams. The functions of an object M appear as directed edges after "decomposition into functions".

constructing the abstract block diagram of a system [84, 85]. Abstract block diagrams contain other structures (e.g. products) but here we only consider the idea of "decomposition into functions" which we believe is central. A simple example of the idea is shown in Figure 2.1. On the left hand side of the picture, M represents a black box (an enzyme, a machine, etc.) that transforms input x into two outputs y and z. On the right hand side of the picture M is decomposed into two functions. The one labeled m_1 transforms x into y and the other, labeled m_2, transforms x into z. Note that the second graph is dual to the first: x, y and z are directed edges of a graph before "decomposition into functions" while they are nodes of a graph after the transformation.

The other idea we consider in this chapter is the operation which is the inverse of "decomposition into functions": that is, the construction of an object by gluing its functions. This idea is found in [75]. Paton represents a system by a pair of undirected graphs called a star graph and a tetrahedron graph (Figure 2.2). The star graph is the extent part of the pair. In the ecosystem example in Figure 2.2, the nodes of the star graph are the names of concrete agents in the real world, like plants, animals, bacteria and so on. Their roles label the edges. Note that objects belonging to different levels (e.g. ecosystem and the others) are mixed up in the set of nodes of the star graph. On the other hand, the tetrahedron graph which is the line-graph of the star graph is the intent part. A line-graph of a graph is obtained by making old edges into new nodes and linking two new nodes if they are tied by an old node. The nodes are now named after the verbs on the edges of the star graph, that is, the functional roles of agents in the ecosystem.

We have so far used the term 'function' in a loose way. However, we shall use the term in a formal way hereafter: the function of a node in a graph is connecting a pair of edges. Thus, in our terminology, the functions of nodes in the star graph become edges in the tetrahedron graph. This is the same idea as "decomposition into functions" in abstract block diagrams. In addition to "decomposition into functions", Paton looks at the operation in the other direction: the transformation of the tetrahedron graph into the star graph. Under this operation the ecosystem implicit in the tetrahedron graph is made explicit by gluing its distributed functions. We can find the idea of "gluing functions" as

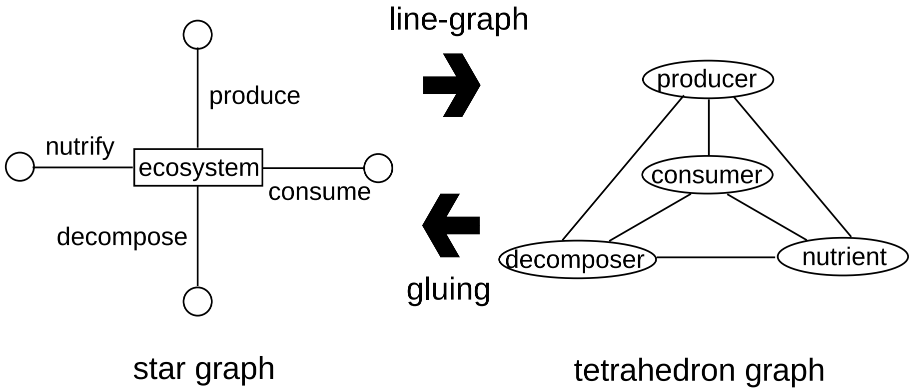

Figure 2.2: Paton's star graph and tetrahedron graph. He describes a concept like an ecosystem by a pair of undirected graphs. The star graph is converted to the tetrahedron graph by making a line-graph. The star graph is produced from the tetrahedron graph by gluing functions.

the inverse operation to "decomposition into functions" in Paton's work. In the following two sections we formalize these two ideas in the category of directed graphs. While Paton's star graph and tetrahedron graph are undirected graphs, we will work in the category of directed graphs for simplicity. The formalization in the category of undirected graphs might become easier after we develop the theory in the category of directed graphs. However, we do not treat that topic in this chapter.

2.3 Decomposition into Functions

We work in the category of directed graphs $\mathcal{G}rph$ in order to formalize the two ideas reviewed in the previous section. The objects in $\mathcal{G}rph$ are directed graphs. (An example of a directed graph is given in Figure 2.3.) A directed graph G consists of a quadruplet $G = (A, O, \partial_0, \partial_1)$ where A is a set of directed edges (or arrows), O is a set of nodes (or objects) and ∂_i $(i = 0, 1)$ are maps from A to O. ∂_0 is a source map that sends each directed edge to its source. ∂_1 is a target map that sends each directed edge to its target. The arrows in $\mathcal{G}rph$ are the homomorphisms of directed graphs. Given directed graphs $G = (A, O, \partial_0, \partial_1)$ and $G' = (A', O', \partial'_0, \partial'_1)$, a homomorphism of directed graphs $D : G \to G'$ consists of two maps $D_O : O \to O'$ and $D_A : A \to A'$ that satisfy the equations $D_O \partial_i = \partial'_i D_A$ $(i = 0, 1)$. As usual, these equations can be represented by the

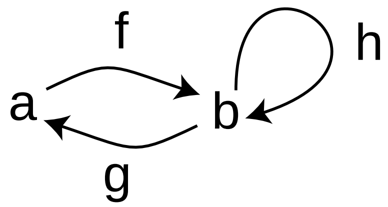

Figure 2.3: An example of a directed graph $G = (A, O, \partial_0, \partial_1)$. The set of directed edges is $A = \{f, g, h\}$. The set of nodes is $O = \{a, b\}$. The source and target maps are defined by $\partial_0 f = a, \partial_1 f = b, \partial_0 g = b, \partial_1 g = a, \partial_0 h = b$ and $\partial_1 h = b$.

following commutative diagram ($i = 0, 1$).

$$\begin{array}{ccc} A & \xrightarrow{D_A} & A' \\ {\scriptstyle \partial_i}\downarrow & & \downarrow{\scriptstyle \partial'_i} \\ O & \xrightarrow{D_O} & O' \end{array}$$

Here we merely consider the functions of a node to be the connection of directed edges. Then the result of the operation of 'decomposition into function' is the so called directed line-graph of a directed graph. This can be seen as a functor from $\mathcal{G}rph$ to itself.

Definition 2.1 *Let R be an operation that transforms given directed graph $G = (A, O, \partial_0, \partial_1)$ into a new directed graph $RG = (RA, RO, \partial_0^R, \partial_1^R)$ by taking its line-graph, where*

$$\begin{aligned} RA &= \{(f, g) \in A \times A | \partial_1 f = \partial_0 g\} \\ RO &= A \\ \partial_0^R(f, g) &= f \ \textit{and} \quad \partial_1^R(f, g) = g \ \textit{for} \ (f, g) \in RA. \end{aligned}$$

It is straightforward to verify that R is an endofunctor (i.e. a functor from $\mathcal{G}rph$ to itself).

The functions of a node in G that connect directed edges become multiple directed edges of RG. For example, node x in Figure 2.4 connects f to h, f to i, g to h and g to i. These functions become four directed edges in RG.

As described above, "decomposition into functions" can be formalized as a functor on $\mathcal{G}rph$. In the next section we also formalize "gluing functions" as a functor on $\mathcal{G}rph$.

2.4 Gluing Functions

A functor that represents "gluing functions" would be a kind of inverse operation to R. Under the operation of R directed edges become nodes. Therefore,

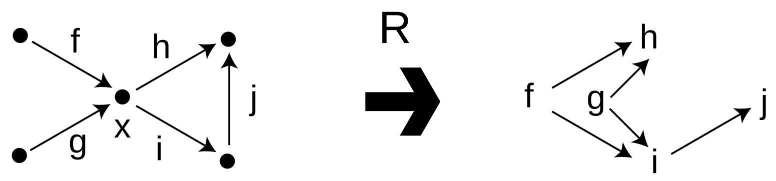

Figure 2.4: The directed edges f, g, h, i and j become nodes under the operation of R. While the node x is decomposed into four directed edges.

a new node created by the operation of "gluing functions" would be obtained by gluing the distributed functions on directed edges.

Motivated by the above consideration, we formalize the inverse operation to R as follows. Given a directed graph $G = (A, O, \partial_0, \partial_1)$, an operation L'' constructs a new directed graph $L''G = (L''A, L''O, \partial_0^{L''}, \partial_1^{L''})$ as follows.

$$\begin{aligned} L''A &= O \\ L''O &= T/\sim'' \\ T &= \{(x, y) \in O \times O | \exists f \in A \; \partial_0 f = x, \partial_1 f = y\} \end{aligned}$$

Here $\sim''$ is an equivalence relation generated by the relation R'' on T defined by

$$(x, y)R''(z, w) \Leftrightarrow x = z \text{ or } y = w.$$

The motivation for the definition of R'' is explained schematically in Figure 2.5. We might expect the source and target maps for $x \in L''A = O$ to be defined by

$$\partial_0^{L''} x = [(\partial_0 f, \partial_1 f)]_{\sim''} \quad \text{and } \partial_1^{L''} x = [(\partial_0 g, \partial_1 g)]_{\sim''}$$

where $\partial_1 f = x, \partial_0 g = x,\ f, g \in A$ and $[\alpha]_{\sim''}$ is the equivalence class that includes α. However, there does not necessarily exist an $f \in A$ such that $\partial_1 f = x$ (or a $g \in A$ such that $\partial_0 g = x$) for all $x \in O$. The problem is that we cannot define a source map for x with 0 in-degree and cannot define a target map for x with 0 out-degree.

There are at least two possible strategies for coping with the problem:

(I) Modifying $L''O$ while keeping the category $\mathcal{G}rph$.

(II) Restricting the category in which we work while maintaining the construction of $L''O$.

In the first strategy we have to modify $L''O$ so that source and target maps work for x with 0 in-degree or 0 out-degree. As we will see below, the idea of "gluing functions" becomes implicit in the first strategy. On the other hand the idea of "gluing functions" remains explicit in the second strategy. In this

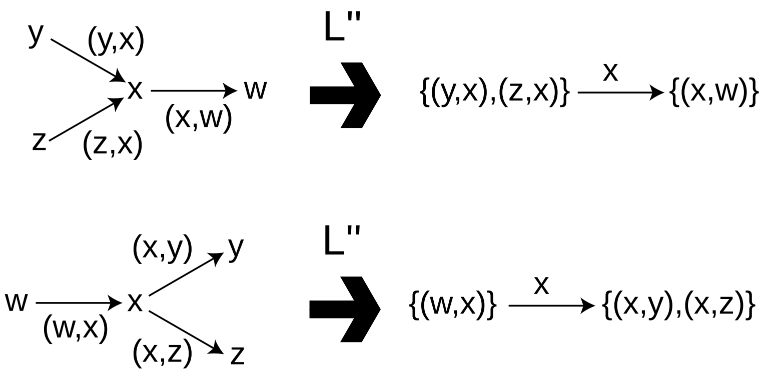

Figure 2.5: Because (y, x) and (z, x) have the same target x, they must be equivalent when x becomes a directed edge (above). Because (x, y) and (x, z) have the same source x, they must be equivalent when x becomes a directed edge (below).

strategy we find the largest subcategory in which L'' becomes a functor. Because we are interested in the duality between "decomposition into functions" and "gluing functions", our emphasis is on the second strategy. Nevertheless, it is also convenient to work following the first strategy. For this reason, we begin by formalizing the first strategy.

Our problem is to modify the definition of $L''O$ so that source and target maps can be defined on all x including 0 in-degree and 0 out-degree nodes. A solution can be obtained by extending the set T which appears in the definition of $L''O$. T is a set of functions which connect two directed edges. The definition of T mentioned above ignores situations in which there are no incoming directed edges to a node or no outgoing directed edges from a node. Hence we add new elements to T to represent the source or target of such edges.

Definition 2.2 *We construct a new directed graph* $L'G = (L'A, L'O, \partial_0^{L'}, \partial_1^{L'})$ *from a given directed graph* $G = (A, O, \partial_0, \partial_1)$ *as follows.*

$$\begin{aligned} L'A &= O \\ L'O &= S/\sim' \\ S &= T \cup (O \times 2) \\ T &= \{(x, y) \in O \times O | \exists f \in A \ \partial_0 f = x, \partial_1 f = y\} \end{aligned}$$

Here $\sim'$ *is an equivalence relation on* S *generated by the following relation* R' *on* S.

$(x, y)R'(z, w) \Leftrightarrow x = z$ *or* $y = w, (x, y)R'(z, 0) \Leftrightarrow y = z, (x, y)R'(z, 1) \Leftrightarrow x = z$

The source and target maps are

$$\partial_0^{L'} x = [(x, 0)]_{\sim'} \quad \text{and } \partial_1^{L'} x = [(x, 1)]_{\sim'}.$$

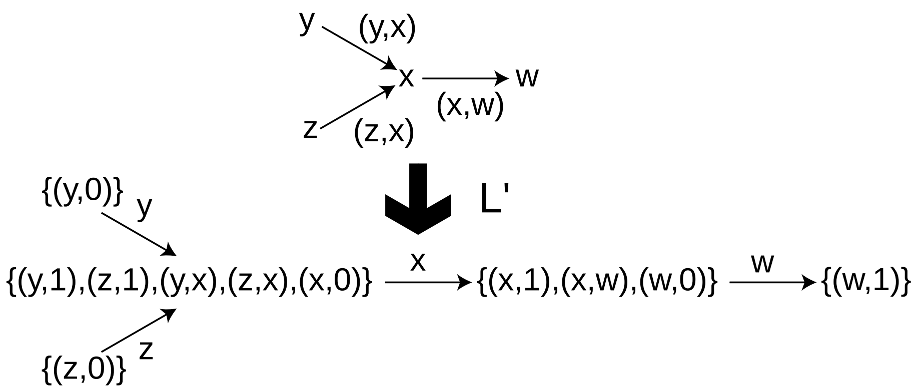

Figure 2.6: An example of the operation of L'. We can define the source and target maps for any new directed edges (unlike L'').

It can be verified that L' is a functor from $\mathcal{G}rph$ to itself.

We can define a functor L that is naturally isomorphic to L' without T (see Figures 2.6 and 2.7). The objects (y, x) and (z, x) in the source of x and (x, w) in the target of x in Figure 2.6 are redundant. We can obtain the same graph without them (see Figure 2.7).

Definition 2.3 *A functor L from $\mathcal{G}rph$ to itself that sends a directed graph $G = (A, O, \partial_0, \partial_1)$ to a directed graph $LG = (LA, LO, \partial_0^L, \partial_1^L)$ is defined as follows.*

$$\begin{aligned} LA &= O \\ LO &= (O \times 2)/\sim \end{aligned}$$

Here $\sim$ is an equivalence relation on $O \times 2$ generated by the relation R on $O \times 2$.

$$(x, 1)R(y, 0) \Leftrightarrow \exists f \in A\ \partial_0 f = x, \partial_1 f = y.$$

The source and target maps are the same as those of L'.

$$\partial_0^L x = [(x, 0)]_\sim \quad \textit{and } \partial_1^L x = [(x, 1)]_\sim$$

Proposition 2.4 *The two functors L and L' are naturally isomorphic.*

Proof. A natural isomorphism $\psi : L \to L'$ is defined as follows. For each directed graph $G = (A, O, \partial_0, \partial_1)$, $\psi_G : LG \to L'G$ consists of two maps. The arrow part is defined by $(\psi_G)_A := id_O : (LG)_A = O \to (L'G)_A = O$. The object part $(\psi_G)_O : (LG)_O \to (L'G)_O$ is defined by sending $[(x, i)]_\sim$ to $[(x, i)]_{\sim'}$ for $i = 0, 1$. $(\psi_G)_O$ is a well-defined map because $(x, 1)R(y, 0) \Leftrightarrow (x, 1)R'^{-1}(x, y)R'(y, 0)$. Bijectivity and naturality can easily be checked. □

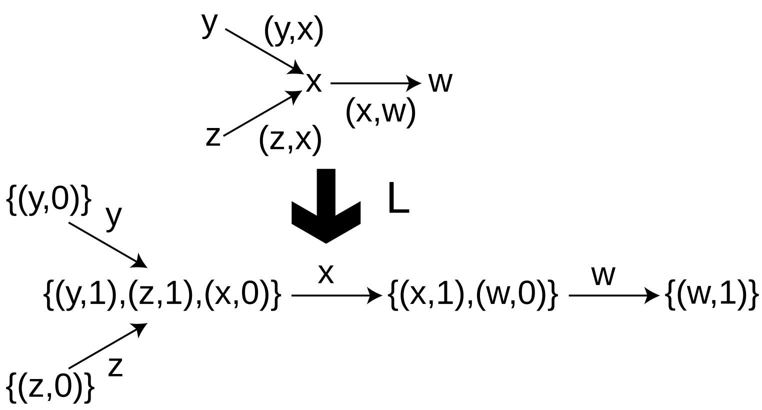

Figure 2.7: L' can be simplified.

2.5 The Adjunctions and its Invariant Structures

In the previous two sections, we defined two functors R and L. L is constructed as the inverse operation of R in some sense. In this section we reveal the precise mathematical meaning of 'inverse'. In fact they are not inverses of each other in the precise meaning of the word but they form an adjunction on $\mathcal{G}rph$. In particular, L is a left adjoint functor to R.

Theorem 2.5 *L is a left adjoint to R. That is, we have a natural isomorphism*

$$\mathcal{G}rph(LG, G') \cong \mathcal{G}rph(G, RG')$$

for any pair of directed graphs G, G'.

Proof. First we construct a map $\varphi_{G,G'} : \mathcal{G}rph(LG, G') \to \mathcal{G}rph(G, RG')$ where $G = (A, O, \partial_0, \partial_1)$ and $G' = (A', O', \partial'_0, \partial'_1)$. Given a directed graph homomorphism $D : LG \to G'$, we have two maps $D_O : LO \to O'$ and $D_A : LA = O \to A'$. We define a directed graph homomorphism $\varphi_{G,G'}(D) : G \to RG'$ from these maps. For the object part we define

$$\varphi_{G,G'}(D)_O := D_A : O \to RO' = A'.$$

For the arrow part

$$\varphi_{G,G'}(D)_A : A \to RA' = \{(f, g) \in A' \times A' | \partial'_1 f = \partial'_0 g\}$$

is defined as a map that sends each $f \in A$ to $(D_A\partial_0 f, D_A\partial_1 f)$. In order to verify $(D_A\partial_0 f, D_A\partial_1 f) \in RA'$, we have to show that $\partial'_1 D_A\partial_0 f = \partial'_0 D_A\partial_1 f$. This result is obtained by the following calculation.

$$\begin{aligned} \partial'_1 D_A \partial_0 f &= D_O \partial^L_1 \partial_0 f \\ &= D_O[(\partial_0 f, 1)]_\sim = D_O[(\partial_1 f, 0)]_\sim \\ &= D_O \partial^L_0 \partial_1 f = \partial'_0 D_A \partial_1 f. \end{aligned}$$

Next we define the inverse map of $\varphi_{G,G'}$, that is, $\varphi^{-1}_{G,G'} : \mathcal{G}rph(G, RG') \to \mathcal{G}rph(LG, G')$. Let $\hat{D} : G \to RG'$ be a directed graph homomorphism. We need to construct $\varphi^{-1}_{G,G'}(\hat{D}) : LG \to G'$ from $\hat{D}_O : O \to RO = A'$ and $\hat{D}_A : A \to RA'$. The arrow part is defined by

$$\varphi^{-1}_{G,G'}(\hat{D})_A := \hat{D}_O : LA = O \to A'.$$

The object part

$$\varphi^{-1}_{G,G'}(\hat{D})_O : LO \to O'$$

is defined as a map that sends $[(x,0)]_\sim$ to $\partial'_1 \hat{D}_O x$ and $[(y,1)]_\sim$ to $\partial'_0 \hat{D}_O y$. The well-definedness of this map can be verified as follows. It is sufficient to show that if $(x,1)R(y,0)$ then $\partial'_1 \hat{D}_O x = \partial'_0 \hat{D}_O y$. If $(x,1)R(y,0)$ holds then there exists $f \in A$ such that $\partial_0 f = x, \partial_1 f = y$. Therefore, we have

$$\begin{aligned} \partial'_1 \hat{D}_O x &= \partial'_1 \hat{D}_O \partial_0 f \\ &= \partial'_1 \partial^R_0 \hat{D}_A f = \partial'_0 \partial^R_1 \hat{D}_A f \\ &= \partial'_0 \hat{D}_O \partial_1 f = \partial'_0 \hat{D}_O y. \end{aligned}$$

lt is easily verified that $\varphi^{-1}_{G,G'}$ is in fact the inverse of $\varphi_{G,G'}$. Naturality is also a routine calculation. □

This adjunction is essentially the same as the one described by Pultr [80]. However, ours is slightly different to that of Pultr [80] who constructed an adjunction between $\mathcal{G}rph$ and the category of directed graphs without multiple directed edges.

Now we describe the unit and counit of the adjunction. The unit is a natural transformation $\eta : I \to RL$ where I is the identity functor on $\mathcal{G}rph$. Given a directed graph $G = (A, O, \partial_0, \partial_1)$, we have $LG = (LA = O, LO = (O \times 2)/\sim, \partial^L_0, \partial^L_1)$. Hence RLG consists of the following data.

$$\begin{aligned} RLA &= \{(x,y) \in LA \times LA = O \times O | \partial^L_1 x = \partial^L_0 y \text{ i.e. } (x,1) \sim (y,0)\} \\ RLO &= O \\ \partial^{RL}_0(x,y) &= x \text{ and } \quad \partial^{RL}_1(x,y) = y \end{aligned}$$

The components of the natural transformation $\eta_G : G \to RLG$ are defined by the following two maps.

$$\begin{aligned} (\eta_G)_O = id_O &: O \to RLO = O \\ (\eta_G)_A &: A \to RLA : f \mapsto (\partial_0 f, \partial_1 f) \end{aligned}$$

The counit is also a natural transformation on $\mathcal{G}rph$, $\epsilon : LR \to I$. For a directed graph $G = (A, O, \partial_0, \partial_1)$ we have $RG = (RA = \{(f,g) \in A \times A | \partial_1 f = \partial_0 g\}, RO = A, \partial^R_0, \partial^R_1)$. Hence we find that LRG consists of the following data.

$$\begin{aligned} LRA &= RO = A \\ LRO &= (RO \times 2)/\sim = (A \times 2)/\sim \\ \partial^{LR}_i f &= [(f,i)]_\sim \ (i = 0,1) \end{aligned}$$

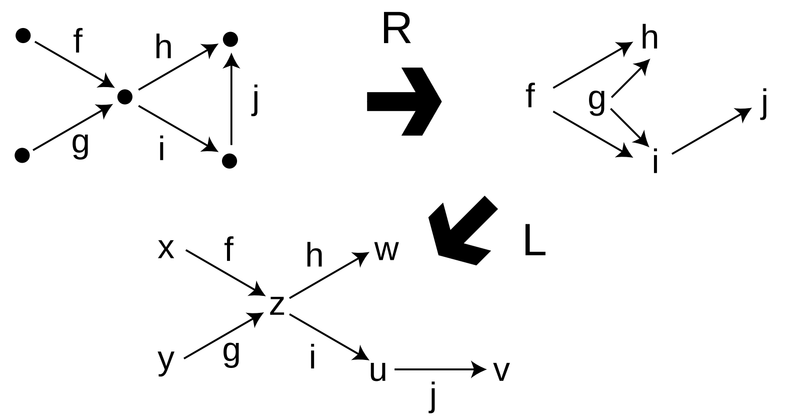

Figure 2.8: Sequential operations of first R and second L. Directed edges h and j have the same target at first. However, after the operation of LR, this target is divided into w and v. Here $x = \{(f,0)\}, y = \{(g,0)\}, z = \{(f,1),(g,1),(h,0),(i,0)\}, w = \{(h,1)\}, u = \{(i,1),(j,0)\}$ and $v = \{(j,1)\}$.

Here $\sim$ is an equivalence relation on $A \times 2$ generated by the relation defined by

$$\begin{aligned} (f,1)R(g,0) \quad &\Leftrightarrow \quad \exists\, \alpha \in RA\ (\partial_0^R \alpha = f, \partial_1^R \alpha = g) \\ &\Leftrightarrow \quad \partial_1 f = \partial_0 g \end{aligned}$$

Each component $\epsilon_G : LRG \to G$ is defined by

$$\begin{aligned} (\epsilon_G)_A = id_A \quad &: \quad LRA = A \to A \\ (\epsilon_G)_O \quad &: \quad LRO = (A \times 2)/\sim \to O : [(f,i)]_\sim \mapsto \partial_i f\ \ (i = 0,1). \end{aligned}$$

The map $(\epsilon_G)_O$ is well-defined because $(f,1)R(g,0) \Leftrightarrow \partial_1 f = \partial_0 g$ as shown above.

The unit and the counit are not natural isomorphisms in general. (An example for the counit is shown in Figure 2.8.) However, directed graphs that are biologically interesting might be those G such that $\eta_G : G \cong RLG$ or $\epsilon_G : LRG \cong G$. That is, if $\eta_G : G \cong RLG$ holds for a directed graph G then G is invariant under the sequential operations of first “gluing functions” and second “decomposition into functions”. On the other hand, if $\epsilon_G : LRG \cong G$ holds then G is invariant under the sequential operations of first “decomposition into functions” and second “gluing functions”. Hence, we consider the conditions for η_G or ϵ_G to be natural isomorphisms in what follows.

Let $G = (A, O, \partial_0, \partial_1)$ be a directed graph. First we consider η_G. Because $(\eta_G)_O$ is an identity we only need the conditions for $(\eta_G)_A$. We write $x \to y$ if there exists a directed edge from x to y.

Lemma 2.6 *Consider the following two conditions.*

(i-a) For $f, g \in A$ if $\partial_i f = \partial_i g$ $(i = 0, 1)$ then $f = g$. That is, there is at most one directed edge between each pair of nodes.

(i-b) If $x \to y, z \to y, z \to w$ then $x \to w$.

Then $(\eta_G)_A$ is injective if and only if condition (i-a) holds and $(\eta_G)_A$ is surjective if and only if (i-b) holds. Condition (i-b) is depicted in Figure 2.9.

Proof. For the injective part,

$$\begin{aligned} (\eta_G)_A \text{ is an injection} \quad &\Leftrightarrow \quad \text{if } (\eta_G)_A(f) = (\eta_G)_A(g) \text{ then } f = g \\ &\Leftrightarrow \quad \text{if } (\partial_0 f, \partial_1 f) = (\partial_0 g, \partial_1 g) \text{ then } f = g \\ &\Leftrightarrow \quad \text{condition (i-a) holds.} \end{aligned}$$

For the subjective part, we first prove necessity. Suppose $(\eta_G)_A$ is a surjection. Then there exists $f \in A$ such that $(\eta_G)_A(f) = (x, y)$ for any $(x, y) \in O \times O$ with $(x, 1) \sim (y, 0)$. That is, if $(x, 1) \sim (y, 0)$ holds then $x \to y$. Suppose $x \to y, z \to y$ and $z \to w$ hold. Then we have $(x, 1)R(y, 0)R^{-1}(z, 1)R(w, 0)$. Hence $(x, 1) \sim (w, 0)$ holds. By the condition for surjectivity we have $x \to w$. This is condition (i-b).

Next we show sufficiency. Suppose condition (i-b) holds. In order to prove that $(\eta_G)_A$ is a surjection, we have to show the existence of $f \in A$ such that $(\eta_G)_A(f) = (x, y)$ for any $(x, y) \in RLA$. This is equivalent to showing that if $(x, 1) \sim (y, 0)$ then $x \to y$. If $(x, 1) \sim (y, 0)$ holds then there exist $s_1, \cdots, s_n \in O \times 2$ such that $(x, 1) = s_1, s_i R \cup R^{-1} s_{i+1}, s_n = (y, 0)$ $(i = 1, 2, \cdots, n-1)$. Because we have $s_1 = (x, 1), s_n = (y, 0)$, the chain must be $s_1 R s_2 R^{-1} s_3 R \cdots R s_n$ with R and R^{-1} appearing alternately in the chain. n takes values $n = 2k + 2$ $(k = 0, 1, 2, \cdots)$. If $k = 0$ then the claim is trivial. If $k = 1$ then there exist $x', y' \in O$ such that $(x, 1)R(x', 0)R^{-1}(y', 1)R(y, 0) \Leftrightarrow x \to x', y' \to x', y' \to y$. By condition (i-b) we get $x \to y$. For the general case, the claim can be verified by mathematical induction. $\square$

Now we consider the counit. Because $(\epsilon_G)_A$ is an identity, we only have to obtain the conditions for $(\epsilon_G)_O$.

Lemma 2.7 *Consider the following conditions.*

(ii-a) If $\partial_i f = \partial_i g$ and $f \neq g$ holds then there exists $h \in A$ such that $\partial_{i+1 \bmod 2} h = \partial_i f (= \partial_i g)$.

(ii-b) For any $x \in O$ there exists $f \in A$ such that $\partial_0 f = x$ or $\partial_1 f = x$.

$(\epsilon_G)_O$ is injective if and only if condition (ii-a) holds. $(\epsilon_G)_O$ is surjective if and only if condition (ii-b) holds. Both conditions are depicted in Figure 2.9.

Proof. First we prove the injective part. Suppose condition (ii-a) holds. Given $\alpha, \beta \in (A \times 2)/\sim$ we have to show that if $(\epsilon_G)_O(\alpha) = (\epsilon_G)_O(\beta)$ then $\alpha = \beta$. We have three cases depending on the representative elements of α and β. The first

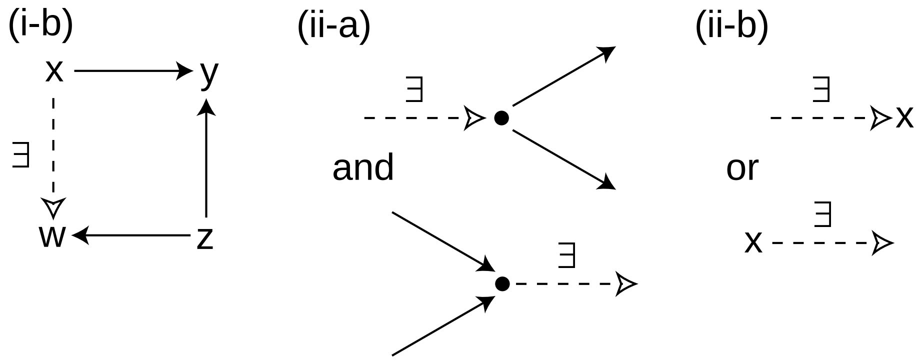

Figure 2.9: The conditions in Lemma 2.6 and Lemma 2.7 are shown schematically.

case we consider is when $\alpha = [(f,1)]_\sim$ and $\beta = [(g,0)]_\sim$. If $(\epsilon_G)_O(\alpha) = (\epsilon_G)_O(\beta)$ holds then we have

$$\partial_1 f = \partial_0 g \Leftrightarrow (f,1)R(g,0) \Rightarrow \alpha = \beta.$$

Next consider the case when α and β have the forms $\alpha = [(f,0)]_\sim$ and $\beta = [(g,0)]_\sim$. If $(\epsilon_G)_O(\alpha) = (\epsilon_G)_O(\beta)$ holds then $\partial_0 f = \partial_0 g$. If $f \neq g$ then there exists $h \in A$ such that $\partial_0 f = \partial_0 g = \partial_1 h$ by condition (ii-a). It follows that $(f,0)R^{-1}(h,1)R(g,0)$. This implies $(f,0) \sim (g,0)$, that is, $\alpha = \beta$. The remaining case $\alpha = [(f,1)]_\sim$ and $\beta = [(g,1)]_\sim$ is similar.

For the opposite direction, suppose $(\epsilon_G)_O$ is an injection. Then $(f,0) \sim (g,0)$ if $\partial_0 f = \partial_0 g$. Hence if $f \neq g$ then there exist $s_1, \cdots, s_n \in A \times 2, (f,0) = s_1 R^{-1} s_2 R \cdots R s_n = (g,0)$. Here n takes values $n = 2k+3$ $(k = 0,1,2,\cdots)$. Because $n \geq 3$, there exist $f,g,h \in A$ such that $(f,0)R^{-1}(h,1) \sim (g,0)$. We get $\partial_0 f = \partial_1 h = \partial_0 g$. Thus we obtain condition (ii-a) for $i = 0$. The condition for $i = 1$ follows similarly.

For surjectivity, if there exists a node that is neither a source nor a target of any directed edge then $(\epsilon_G)_O$ is not a surjection because the value of $(\epsilon_G)_O$ is a source or a target of a directed edge. This proves necessity. For sufficiency, suppose condition (ii-b) holds. Then for any $x \in O$ there exist $i \in \{0,1\}$ and $f \in A$ such that $(\epsilon_G)_O([(f,i)]_\sim) = \partial_i f = x$. Hence $(\epsilon_G)_O$ is a surjection. $\square$

Using Lemma 2.6 and Lemma 2.7, we obtain the following theorem.

Theorem 2.8 *The largest subcategory of $\mathcal{G}rph$ on which the unit $\eta : I \to RL$ is a natural isomorphism consists of directed graphs that satisfy conditions (i-a) and (i-b) and have directed graph homomorphisms between them. This is a full subcategory of $\mathcal{G}rph$. Similarly the full subcategory of $\mathcal{G}rph$ whose objects are directed graphs that satisfy conditions (ii-a) and (ii-b) is the largest subcategory of $\mathcal{G}rph$ on which the counit $\epsilon : LR \to I$ is a natural isomorphism.*

The results for strategy (I) are summarized in Theorem 2.5 and Theorem 2.8. However, the functor L does not represent the idea of "gluing functions" explicitly. In order to give an explicit representation of "gluing functions" as a functor, we must restrict the category in which we work. This is strategy (II) which we consider in what follows. In contrast to the first strategy, we can obtain an explicit adjunction between "decomposition into functions" and "gluing functions". The operation which represents "gluing functions" directly is L'' which was defined in the previous section. First we define the category with which we work hereafter.

Definition 2.9 *A subcategory $\mathcal{H}$ of $\mathcal{G}rph$ is defined as follows.*

The objects in $\mathcal{H}$ are directed graphs $G = (A, O, \partial_0, \partial_1)$ that satisfy the following condition.

(H) For all $x \in O$ there exist $f, g \in A$ such that $\partial_1 f = x = \partial_0 g$.

The arrows in $\mathcal{H}$ are homomorphisms of directed graphs. That is, $\mathcal{H}$ is a full subcategory of $\mathcal{G}rph$.

Condition (H) is the weakest condition under which the operation L'' becomes a functor. This is justified by the following proposition.

Proposition 2.10 *A directed graph $G = (A, O, \partial_0, \partial_1)$ satisfies condition (H) if and only if any equivalence class of $L'O$ includes an element of T, where $T = \{(x, y) \in O \times O | \exists f \in A\ \partial_0 f = x, \partial_1 f = y\}$.*

Proof. Suppose $G = (A, O, \partial_0, \partial_1)$ satisfies condition (H). For any $\alpha \in L'O$ there exist $x \in O$ and $i \in \{0, 1\}$ such that $\alpha = [(x, i)]_{\sim'}$. Consider the case $\alpha = [(x, 0)]_{\sim'}$. By condition (H), there exists $f \in A$ such that $x = \partial_1 f$. We have $(\partial_0 f, \partial_1 f) \in \alpha$ because $(\partial_0 f, \partial_1 f) R' (x, 0)$, where R' is the relation on $S = T \cup (O \times 2)$ given in definition 2.2. The other case can be proved similarly.

For the opposite direction, suppose any $\alpha \in L'O$ includes an element of T. Fix any element $z \in O$. By assumption, there exists $(x, y) \in T$ such that $(z, 0) \sim' (x, y)$. There also exists $(x', y') \in T$ such that $(x', y') R' (z, 0)$. By the definition of R', we have $y' = z$. We obtain $z = \partial_1 f$ for $f \in A$ such that $\partial_0 f = x'$ and $\partial_1 f = y'$. The existence of $g \in A$ such that $z = \partial_0 g$ can be shown in the same way by considering $(x'', y'') \in T$ such that $(x'', y'') R' (z, 1)$. □

Now we collect some facts about $\mathcal{H}$ and L''.

Proposition 2.11 *Let $\mathcal{H}$ be the subcategory defined in Definition 2.9 and let R and L'' be the functors defined in sections three and four respectively. Then*

(i) L'' is a functor from $\mathcal{H}$ to $\mathcal{G}rph$.

(ii) L'' is naturally isomorphic to L on $\mathcal{H}$.

(iii) If a directed graph G satisfies condition (H) then $L''G$ also satisfies (H).

(iv) If a directed graph G satisfies condition (H) then RG also satisfies (H).

Proof.

(i) The proof is a straightforward verification.

(ii) It is sufficient to show that $L'' \cong L'$ on $\mathcal{H}$ because we have $L' \cong L$ on $\mathcal{G}rph$ by Proposition 2.4. We define a natural isomorphism $\phi : L'' \to L'$ as follows. Given a directed graph $G = (A, O, \partial_0, \partial_1)$, the components of ϕ_G are two maps. The arrow part is defined by $(\phi_G)_A := id_O : L''A = O \to L'A = O$. The object part $(\phi_G)_O : L''O \to L'O$ is defined as a map that sends $[(x, y)]_{\sim''}$ to $[(x, y)]_{\sim'}$. This map is well-defined because $(x, y)R''(z, w)$ implies $(x, y)R'(z, w)$.

(iii) For any $[(x, y)]_{\sim''} \in L''O$ there exists $f \in A$ such that $\partial_0 f = x$ and $\partial_1 f = y$. By the definition of source and target maps for $L''G$, we obtain $\partial_1^{L''} x = [(x, y)]_{\sim''} = \partial_0^{L''} y$.

(iv) Take any $f \in RO = A$. There exist $g, h \in A$ such that $\partial_0 f = \partial_1 g$ and $\partial_1 f = \partial_0 h$ by condition (H). Because $(g, f), (f, h) \in RA$, we obtain $\partial_1^R (g, f) = f = \partial_0^R (f, h)$.

□

By Theorem 2.5 and Proposition 2.11, we obtain the following adjunction on $\mathcal{H}$.

Theorem 2.12 *L'' is a left adjoint functor to R on $\mathcal{H}$. That is, we have a natural isomorphism*

$$\mathcal{H}(L''G, G') \cong \mathcal{H}(G, RG')$$

for any pair of directed graphs G, G' in $\mathcal{H}$.

Thus the adjunction in Theorem 2.12 is a restriction of the one in Theorem 2.5 to the subcategory $\mathcal{H}$. Meanwhile, condition (H) implies conditions (ii-a) and (ii-b) in Lemma 2.7. Hence the counit $\epsilon : L''R \to I$ is a natural isomorphism. On the other hand, condition (H) has nothing to do with the proof of the conditions for injectivity and surjectivity of $\eta_G : G \to RL''G$ in Lemma 2.6. Therefore, a necessary and sufficient condition for $\eta_G : G \to RL''G$ to be an injection is condition (i-a) in Lemma 2.6 and the necessary and sufficient condition for surjectivity is condition (i-b) in Lemma 2.6. Summarizing these facts, we obtain the following theorem.

Theorem 2.13 *The counit $\epsilon : L''R \to I$ is a natural isomorphism on $\mathcal{H}$. The full subcategory of $\mathcal{H}$ whose objects are directed graphs satisfying conditions (i-a) and (i-b) is the largest subcategory of $\mathcal{H}$ on which $\eta : I \cong RL''$ holds.*

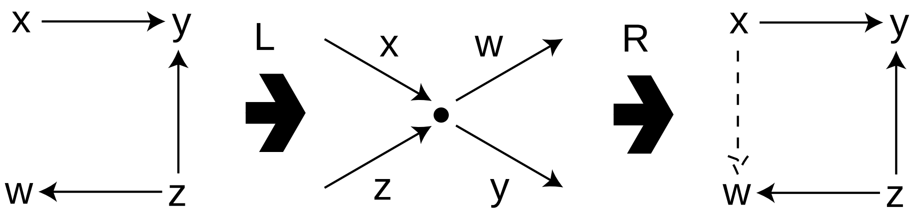

Figure 2.10: A schematic explanation of condition (i-b). Because x and w are tied by a node in the picture in the center, a new directed edge from x to w is made.

2.6 Discussion

In this section we discuss the significance of the adjunctions found in the previous section and their consequences for theoretical biology.

As we have seen above, we have to work in the subcategory $\mathcal{H}$ of $\mathcal{G}rph$ in order to define the idea of "gluing functions" as a functor. Condition (H) means that any directed graph in $\mathcal{H}$ is closed when following arrows either forward or backward. If G is a finite directed graph that satisfies (H) then this implies there exists a cycle in G. Thus we obtain the existence of a cycle in a directed graph as a necessary condition for "gluing functions" to be defined. Furthermore the existence of a cycle is conserved by both L'' and R. In particular, by Theorem 2.13, the same cycle is recovered under the sequential operations of first "decomposition into functions" and second "gluing functions".

Mathematically, a directed graph G is a line-graph of some directed graph if and only if G satisfies conditions (i-a) and (i-b) [80]. However, here we shall consider them from the point of view of theoretical biology.

Condition (i-a) means there is only one directed interaction between two nodes. It seems that this says any node can only be active or passive but not both. However, if we keep in mind that a directed graph is a syntactic representation of a system, this is not such a disappointing condition. A system can still have rich semantic structures. Instead, we can avoid a complicated description of a system by using this constraint.

Condition (i-b) seems mysterious at first sight. However, this is a trivial gluing condition if we make nodes into directed edges. Suppose $x \to y, z \to y$ and $z \to w$. If we operate with L on a directed graph that consists of four nodes and the described directed edges, we obtain a directed graph with one node and two incoming edges x, z and two outgoing edges y, z. Before the operation of L, there are three links from x to y, from z to y and from z to w. However, After the operation of L, a new link from x to w is generated. Graphically, this is obvious (see Figure 2.10). Actually we obtain a new directed edge from x to w by operating with R.

Condition (i-b) can be seen from another point of view. It can be interpreted

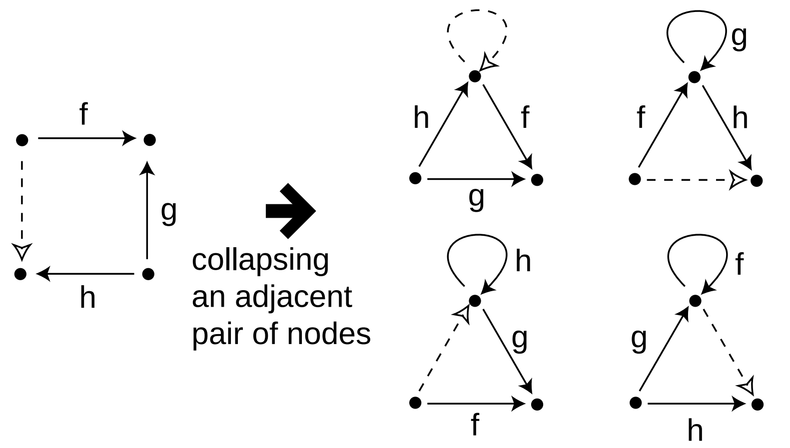

Figure 2.11: Under condition (i-b) the square graph of Figure 2.10 becomes one of four diagrams whose shapes are the same (triangle with a loop) if one of directed edges in the square is made into a loop. The four diagrams can be seen as anticipatory diagrams.

as a diagram for anticipation. Here we use the term anticipation in the sense of making a link between two things from some clues. This becomes visible by collapsing an adjacent pair of nodes in the square graph (Figure 2.11). All four diagrams on the right hand side of Figure 2.11 have the same shape. Only the position of the broken arrow is different, depending on which pair of nodes is collapsed. The square diagram is the least graph which unifies the four triangular diagrams. Let us examine the upper right diagram. This diagram says that f and h are 'composable' if there exists a loop g. (Assume that there exists at most one directed edge between two nodes, that is, condition (i-a) also holds.) The role of g is to link the target of f and the source of h. Edges f and h cannot be composed without g. A link between the source of f and the target of h is 'anticipated' by g. In the upper left diagram the broken loop which links the target of h and the source of f is 'anticipated' by the commutative triangle. In the lower left and lower right diagrams the commutative triangle is completed by the linking action of a loop. As observed above, the construction of the commutative triangle involves a linkage between the upper left edge and the upper right edge. We can regard this as a representation of anticipation in the sense given above.

2.7 Summary and Outlook

In this chapter we have developed an adjunction between "decomposition into functions" and "gluing functions" in the category of directed graphs. The existence of a cycle and anticipatory diagrams are obtained as implications from the invariant structures of the adjunction. This is a new derivation of these significant conditions for theoretical biology.

We here propose two directions for future research not described in this thesis. The first is the study of the gluing closure which is derived from the unit of adjunction $\eta : I \to RL$. Let X be a set and R be a relation on X. (X, R) can be seen as a directed graph with X as the set of nodes and $R \subset X \times X$ as the set of directed edges. This is a directed graph without multiple directed edges. Let R_2 be a binary relation on $X \times 2$ defined by $(x, 1)R_2(y, 0) \Leftrightarrow xRy$ and let $\sim$ be the equivalence relation on $X \times 2$ generated by R_2. We define the gluing closure of R by

$$\overline{R} := \{(x, y) \in X \times X | (x, 1) \sim (y, 0)\}.$$

In particular, studying the gluing closure on random graphs would provide an insight into the effects of "gluing functions" from the statistical point of view.

The second direction is the mathematical formalization of Ray Paton's idea. As described in section two he represents a concept by a pair of graphs, the star graph and the tetrahedron graph. We pointed out that the star graph is an extent part and the tetrahedron graph is an intent part. His idea seems to be generalizable as a formal concept analysis (FCA) [20] on $\mathcal{G}rph$. Because $\mathcal{G}rph$ can be viewed as a topos [53, 113], everything in FCA can be generalized trivially in $\mathcal{G}rph$. However, so called polar operations become uninteresting in such a trivial generalization. Because Paton's idea includes the adjunction described in this chapter, a generalization in relation to the adjunction might be needed. We expect that we can obtain a mathematical framework that describes collective concepts (e.g. ecosystem, protein, family, army and so on) because the node set of a graph can include objects belonging to different levels.

In relation to collective concepts, the problem of the coherence of parts to be glued is a significant issue in real biological phenomena [28, 61]. A concept for the foundation of coherence has been proposed: it is called material cause by Gunji et al. [28] and quantum by Matsuno [61]. However, it seems difficult to treat the problem of coherent gluing in the proposed framework because the process of gluing treated in this chapter is a logical process that has no time dependent aspect: the gluing is performed in a single operation. In order to make a link between the proposed framework and these concepts, we must think carefully about what is represented by a graph.

There are at least three different ways to look at a graph. The first way involves a local perspective. A directed edge between two nodes expresses a causal sequence. This is a local structure of a graph and a whole graph is a disjoint sum of such structures. The second way of looking involves a global perspective. A graph represents the time-independent relational structure of a system. The third perspective is a compromise between the first and the second. On the one hand uncoordinated causal sequences proceed in parallel, on the other they are coherently glued as a whole. The framework used in this chapter is apparently based on the second perspective. It would not be until the third perspective is formalized in the language of graphs that the problem of the coherent gluing of parts can be treated. We will return to this problem in chapter 5.

2.8 Another Formulation of the Duality

In the main text we formalize "decomposition into functions" as a functor from $\mathcal{G}rph$ to itself that sends each directed graph to its line-graph. However, we can see the construction of the line-graph from a given directed graph in a different way. It can be formalized as a functor from $\mathcal{G}rph$ to the category of two-dimensional directed graphs $2\mathcal{G}rph$. This functor also has a left adjoint. We construct this adjunction in this appendix.

Let Γ be the category defined by the following diagram.

$$C_2 \underset{t_1}{\overset{s_1}{\leftleftarrows}} C_1 \underset{t_0}{\overset{s_0}{\leftleftarrows}} C_0$$

The category of two-dimensional directed graphs is defined as the presheaf category $2\mathcal{G}rph := \mathcal{S}ets^{\Gamma^{op}}$. We define a functor $R : \mathcal{G}rph \to 2\mathcal{G}rph$ that sends each directed graph $G = A_1 \underset{\partial_{0,1}}{\overset{\partial_{0,0}}{\rightrightarrows}} A_0$ to

$$RG \quad = \quad \{(f,g) \in A_1 \times A_1 | \partial_{0,1} f = \partial_{0,0} g\} \underset{\partial^R_{1,1}}{\overset{\partial^R_{1,0}}{\rightrightarrows}} A_1 \underset{\partial^R_{0,1}}{\overset{\partial^R_{0,0}}{\rightrightarrows}} A_0.$$

The source and target maps are defined by $\partial^R_{1,0}(f,g) = f, \partial^R_{1,1}(f,g) = g, \partial^R_{0,i} = \partial_{0,i}\ \ (i = 0,1)$. $R : \mathcal{G}rph \to 2\mathcal{G}rph$ transforms a given directed graph into a line graph.

An inverse functor $L : 2\mathcal{G}rph \to \mathcal{G}rph$ is defined by sending $G = A_2 \underset{\partial_{1,1}}{\overset{\partial_{1,0}}{\rightrightarrows}} A_1 \underset{\partial_{0,1}}{\overset{\partial_{0,0}}{\rightrightarrows}} A_0$ to

$$A_1 \underset{\partial^L_{0,1}}{\overset{\partial^L_{0,0}}{\rightrightarrows}} A_0/\sim,$$

where $\sim$ is the equivalence relation generated by the relation R on A_0 defined by

$$xRy \Leftrightarrow \exists \alpha \in A_2\ \exists f,g \in A_1\ \partial_{1,0}\alpha = f, \partial_{1,1}\alpha = g, \partial_{0,1} f = x, \partial_{0,0} g = y.$$

The source and target maps are $\partial^L_{0,i} f = [\partial_{0,i} f]_\sim\ (i = 0,1)$. L glues zero-dimensional arrows so that two-dimensional arrows represent links between two one-dimensional arrows such that the target of one is tied to the source of the other.

We, therefore, have the following adjunction.

Theorem 2.14 *For any two-dimensional directed graph G and directed graph G', we have a natural isomorphism*

$$\mathcal{G}rph(LG, G') \cong 2\mathcal{G}rph(G, RG').$$

Proof. We only describe the construction of the bijection. Put $G = A_2 \underset{\partial_{1,1}}{\overset{\partial_{1,0}}{\rightrightarrows}} A_1 \underset{\partial_{0,1}}{\overset{\partial_{0,0}}{\rightrightarrows}} A_0$ and $G' = A'_1 \underset{\partial'_{0,1}}{\overset{\partial'_{0,0}}{\rightrightarrows}} A'_0$. First we define a map $\varphi_{G,G'} : \mathcal{G}rph(LG, G') \to 2\mathcal{G}rph(G, RG')$. Suppose $D : LG \to G'$ is given. We have two maps $D_1 : A_1 \to A'_1$ and $D_0 : A_0/\sim \to A'_0$. The zero-dimensional and one-dimensional parts of $\varphi_{G,G'}(D)$ are defined by

$$\begin{array}{rcl} \varphi_{G,G'}(D)_0 & : & A_0 \to A'_0 : x \mapsto D_0([x]_\sim) \\ \varphi_{G,G'}(D)_1 := D_1 & : & A_1 \to A'_1. \end{array}$$

The two-dimensional part

$$\varphi_{G,G'}(D)_2 : A_2 \to \{(f,g) \in A'_1 \times A'_1 | \partial'_{0,1} f = \partial'_{0,0} g\}$$

is as follows. Given $\alpha \in A_2$, we have $(\partial_{1,0}\alpha, \partial_{1,1}\alpha) \in A_1 \times A_1$ and $(D_1\partial_{1,0}\alpha, D_1\partial_{1,1}\alpha) \in A'_1 \times A'_1$. We define $\varphi_{G,G'}(D)_2(\alpha) := (D_1\partial_{1,0}\alpha, D_1\partial_{1,1}\alpha)$. We have to check $\partial'_{0,1}D_1\partial_{1,0}\alpha = \partial'_{0,0}D_1\partial_{1,1}\alpha$. This result is obtained by the following calculation. We have

$$\partial'_{0,1}D_1\partial_{1,0}\alpha = D_0\partial^L_{0,1}\partial_{1,0}\alpha = D_0([\partial_{0,1}\partial_{1,0}\alpha]_\sim)$$

and

$$\partial'_{0,0}D_1\partial_{1,1}\alpha = D_0\partial^L_{0,0}\partial_{1,1}\alpha = D_0([\partial_{0,0}\partial_{1,1}\alpha]_\sim).$$

Because $\partial_{0,1}\partial_{1,0}\alpha R \partial_{0,0}\partial_{1,1}\alpha$, the right hand sides are identical.

Next we describe $\varphi^{-1}_{G,G'} : 2\mathcal{G}rph(G, RG') \to \mathcal{G}rph(LG, G')$. For any $\hat{D} : G \to RG'$ we have three maps $\hat{D}_2 : A_2 \to \{(f,g) \in A'_1 \times A'_1 | \partial'_{0,1} f = \partial'_{0,0} g\}$, $\hat{D}_1 : A_1 \to A'_1$ and $\hat{D}_0 : A_0 \to A'_0$. The one-dimensional part of $\varphi^{-1}_{G,G'}(\hat{D})$ is defined by

$$\varphi^{-1}_{G,G'}(\hat{D})_1 := D_1 : A_1 \to A'_1.$$

The zero-dimensional part

$$\varphi^{-1}_{G,G'}(\hat{D})_0 : A_0/\sim \to A'_0$$

is defined by $\varphi^{-1}_{G,G'}(\hat{D})_0([x]_\sim) := \hat{D}_0(x)$ for $x \in A_0$. In order to check the well-definedness of $\varphi^{-1}_{G,G'}$, it is sufficient to show that if xRy then $\hat{D}_0(x) = \hat{D}_0(y)$.

Suppose xRy then there exist $\alpha \in A_2$ and $f, g \in A_1$ such that $\partial_{1,0}\alpha = f, \partial_{1,1}\alpha = g, \partial_{0,1}f = x$ and $\partial_{0,0}g = y$. We have

$$\hat{D}_0(x) = \hat{D}_0\partial_{0,1}f = \partial'_{0,1}\hat{D}_1 f = \partial'_{0,1}\hat{D}_1\partial_{1,0}\alpha = \partial'_{0,1}\partial^R_{1,0}\hat{D}_2\alpha$$

and

$$\hat{D}_0(y) = \hat{D}_0\partial_{0,0}g = \partial'_{0,0}\hat{D}_1 g = \partial'_{0,0}\hat{D}_1\partial_{1,1}\alpha = \partial'_{0,0}\partial^R_{1,1}\hat{D}_2\alpha.$$

By the definition of the codomain of $\hat{D}_2$ the right hand sides must be identical.
$\square$

Chapter 3

Wholeness and Information Processing in Biological Networks: An Algebraic Study of Network Motifs

In this chapter we address network motifs found in information processing networks in nature. Network motifs are local structures in a whole network on one hand, they are materializations of a kind of wholeness to have biological functions on the other hand. We formalize the wholeness by the notion of sheaf. We also formalize a feature of information processing by considering an internal structure of nodes. We obtain network motifs bi-fan (BF) and feed-forward loop (FFL) by purely algebraic considerations. We can interpret them as the result of stabilization of a specific information processing pattern, which we call intrinsic motif.

3.1 Introduction

Network motifs are local structures found in various biological networks more frequently than random graphs with the same number of nodes and degrees [65, 66]. They are considered to be units of biological functions [3]. Their significance in biological networks such as gene transcription regulations, protein-protein interactions and neural networks are widely discussed (e.g. [3] and references therein). In general, what kinds of network motifs are found depends on the nature of biological networks. However, some common motifs are found in different kinds of biological networks. In particular, motifs called feed-forward loop (FFL) and bi-fan (BF) are common in both gene transcription regulation networks and neural networks [65]. It is pointed out that both networks are information processing networks [65]. There is already an explanation by selection about what kinds of motifs arise [101], however, the relationship between motifs and information processing is not yet clear.

In this chapter, we investigate the relationship between motifs and information processing by abstract algebra such as theories of sheaves, categories and topoi [52, 53]. It is crucial to represent motifs and information processing by suitable ways. Our formalism is based on two simple ideas. The first idea is that although motifs are local structures in a whole network, motifs themselves are coherent wholes to have biological functions. This fact is formalized as a condition related to sheaves, in which coherent parts are glued uniquely as a whole. The second idea is that in information processing networks each node has two roles, receiver and sender of information. Information is processed between reception and sending. Therefore nodes in information processing networks can be considered to have an internal structure. We assume a simple internal structure and formalize it by so-called Grothendieck construction.

This chapter is organized as follows. In section 2, the idea that motifs as coherent wholes are formalized by sheaves. However, we will see that no interesting consequence can be derived by only this idea. In section 3, we assume that each node of a network has information processing ability and their hypothetical simple internal structure is presented. Integrating this idea and the idea described in section 2, we derive network motifs FFL and BF as conditional statements. Finally in section 4, we give conclusions.

3.2 Motifs as coherent wholes

The basic structure of networks is just a correspondence between a set of nodes and a set of arrows. Finding motifs in a given network implies introduction of a kind of wholeness. Nodes and arrows in a motif make a coherent whole. In this section we describe this wholeness mathematically.

All networks in this chapter are assumed to be directed graphs. A directed graph G consists of a quadruplet $(A, O, \partial_0, \partial_1)$. A is a set of arrows and O is a set of nodes. ∂_0, ∂_1 are maps from A to O. ∂_0 is a source map that sends each arrow to its source node. ∂_1 is a target map that sends each arrow to its target node. A network motif is given by a directed graph $M = (M_A, M_O, \partial_0^M, \partial_1^M)$. We assume that for any node $x \in M_O$ there exists an incoming arrow to x or an outgoing arrow from x. The category of directed graph $\mathcal{G}rph$ is defined as follows. Objects are directed graphs and morphisms are homomorphisms of directed graphs.

Let G be a directed graph that represents a network in nature. Given a motif M, we would like to find all local structures found in G that are the same as M. How they can be described mathematically? First let us concern nodes and arrows as local structures of directed graphs. The set of nodes in G can be identified with the set of homomorphisms of directed graphs from the trivial directed graph consisting of a single node without arrows $\{*\}$ to G

$$\mathrm{Hom}(\{*\}, G).$$

As the same way, the set of arrows in G can be identified with the set of homomorphisms of directed graphs from the directed graph with two distinct nodes and a single arrow between them $\{n_0 \to n_1\}$ to G

$$\mathrm{Hom}(\{n_0 \to n_1\}, G).$$

By the analogy with the above identifications, we define the set of all local structures in G that are the same as M by the set of homomorphisms of directed graphs from M to G

$$\mathrm{Hom}(M, G).$$

The above three Hom's can be treated at the same time by the technique called Grothendieck construction. We describe this in the next subsection.

3.2.1 Grothendieck Construction

Let M be a motif. We define a finite category $\mathcal{C}_M$ as follows. We have three objects $0, 1, 2$. The set of morphisms is generated by identities, two morphisms m_0, m_1 from 0 to 1 and morphisms u_f from 1 to 2 for each $f \in M_A$ with a relation $u_f m_i = u_g m_j (i, j \in \{0, 1\})$ when $\partial_i^M f = \partial_j^M g$.

$$0 \underset{m_1}{\overset{m_0}{\rightrightarrows}} 1 \overset{u_f}{\to} 2$$

We define a functor E from $\mathcal{C}_M$ to $\mathcal{G}rph$. The correspondence of objects are defined by

$$E(0) = \{*\},\ E(1) = \{n_0 \to n_1\},\ E(2) = M.$$

The correspondence of morphisms are determined by

$$E(m_0)_O(*) = n_0,\ E(m_1)_O(*) = n_1,\ E(u_f)_A(\to) = f \text{ for } f \in M_A.$$

Here we denote a homomorphism of directed graphs D by a pair of maps $D = (D_A, D_O)$, where D_A is a map between the set of morphisms and D_O is a map between the set of nodes.

The functor E defines a functor R_E from $\mathcal{G}rph$ to the category $\mathcal{S}ets^{\mathcal{C}_M^{op}}$ of presheaves on $\mathcal{C}_M$, where $\mathcal{S}ets$ is the category of sets. Given a directed graph G we define

$$R_E(G) = \mathrm{Hom}(E(-), G).$$

Grothendieck construction [53] says that a tensor product functor is defined as a left adjoint functor to R_E. Here we do not go into general theory but just give a concrete representation of the left adjoint L_E. Let F be a presheaf on $\mathcal{C}_M$. Omitting the calculation, we obtain L_E by

$$L_E(F) = F \otimes_{\mathcal{C}_M} E \cong F(1) \underset{F(m_1)}{\overset{F(m_0)}{\rightrightarrows}} F(0).$$

From this one can see that the composition $L_E R_E$ is isomorphic to the identity functor on $\mathcal{G}rph$. In general, the reverse composition $R_E L_E$ is not isomorphic to the identity functor on $\mathcal{S}ets^{\mathcal{C}_M^{op}}$. However, if we define a suitable Grothendieck topology J_M on $\mathcal{C}_M$ and concern the category of all J_M-sheaves $\mathcal{S}h(\mathcal{C}_M, J_M)$ then the composition $R_E L_E$ can become isomorphic to the identity on $\mathcal{S}h(\mathcal{C}_M, J_M)$. Thus we can obtain an equivalence of categories $\mathcal{S}h(\mathcal{C}_M, J_M) \simeq \mathcal{G}rph$. We describe the topology J_M in the next subsection.

3.2.2 Grothendieck Topologies

By defining a Grothendieck topology J on a small category $\mathcal{C}$, we can obtain a system of covering in $\mathcal{C}$ and consequently address relationships between parts and whole [53]. J sends each object C in $\mathcal{C}$ to a collection $J(C)$ of sieves on C. A set of morphisms S is called *sieve* on C if any $f \in S$ satisfies $\mathrm{cod}(f) = C$ and the condition $f \in S \Rightarrow fg \in S$ holds. Let S be a sieve on C and $h : D \to C$ be any morphism to C. Then $h^*(S) = \{g|\mathrm{cod}(g) = D,\ hg \in S\}$ is a sieve on D. If $R = \{f_i\}_{i\in I}$ is a family of morphisms with $\mathrm{cod}(f_i) = C$ for any $i \in I$ then $(R) = \{fg|\mathrm{dom}(f) = \mathrm{cod}(g),\ f \in R\}$ is a sieve on C.

Definition 3.1 *A Grothendieck topology on a small category $\mathcal{C}$ is a function that sends each object C to a collection $J(C)$ of sieves on C such that the following three conditions are satisfied.*

(i)maximality *$t_C \in J(C)$ for any maximal sieve $t_C = \{f|\mathrm{cod}(f) = C\}$.*

(ii)stability *If $S \in J(C)$ then $h^*(S) \in J(D)$ for any morphism $h : D \to C$.*

(iii)transitivity *For any $S \in J(C)$, if R is any sieve on C and $h^*(R) \in J(D)$ for all $h : D \to C \in S$ then $R \in J(C)$.*

We call a sieve S that is an element of $J(C)$ a *cover* of C.

Let M be a motif and $\mathcal{C}_M$ be the category defined by the previous subsection. We define a Grothendieck topology J_M on $\mathcal{C}_M$ by

$$J_M(0) = \{t_0\},\ J_M(1) = \{t_1\},\ J_M(2) = \{t_2, S_M = (\{u_f\}_{f\in M_A})\}.$$

Indeed, J_M satisfies the above three axioms. First maximality is obvious. Second, stability is satisfied since $v^*(t_i) = t_j$ for any arrow $v : j \to i$ and $v^*(S_M) = t_j$ for any $v : j \to 2$. Finally, for tansitivity, suppose that for any sieve R on i and $v : j \to i \in t_i$, $v^*(R) \in J_M(i)$ holds for each $t_i \in J_M(i)$. By putting $v = id_i$ we obtain $R \in J_M(i)$. For $S_M \in J_M(2)$, suppose that $v^*(R) \in J_M(j)$ holds for any sieve R on 2 and any $v : j \to 2 \in S_M$. By putting $v = u_f$, we obtain

$$u_f^*(R) = \{v|u_f v \in R\} \in J_M(1).$$

Hence $\{v|u_f v \in R\} = t_1$. This implies that $u_f = u_f \mathrm{id}_1 \in R$. Since this holds for any $f \in M_A$, we have $S_M = (\{u_f\}_{f\in M_A}) \subseteq R$, which means $R = S_M$ or $R = t_2$. In both cases $R \in J_M(2)$.

3.2.3 Sheaves

Roughly speaking, sheaves are mechanisms that glue coherent parts into a unique whole [53].

Definition 3.2 *Let $\mathcal{C}$ be a small category and J be a Grothendieck topology on $\mathcal{C}$. Let F be a presheaf on $\mathcal{C}$ and $S \in J(C)$ be a cover of an object C. A matching family of F with respect to S is a function that sends each element $f : D \to C$ of S to an element $x_f \in F(D)$ such that*

$$F(g)x_f = x_{fg}$$

holds for all $g : D' \to D$. An amalgamation for such a matching family is an element $x \in F(C)$ such that

$$F(f)x = x_f$$

for all $f \in S$. A presheaf F on $\mathcal{C}$ is called sheaf with respect to J (in short, J-sheaf) if any matching family with respect to any cover $S \in J(C)$ for any object C has a unique amalgamation.

A sieve S on an object C can be identified with a subfunctor of Yoneda embedding $\mathrm{Hom}(-, C)$. Hence a matching family of a presheaf F with respect to S is a natural transformation $S \to F$. We denote the collection of matching family of F with respect to S by $\mathrm{Match}(S, F)$.

The condition of sheaf can be restated as follows. Given a Grothendieck topology J on a small category $\mathcal{C}$, a presheaf F on $\mathcal{C}$ is J-sheaf if and only if the map

$$\kappa_S : F(C) \to \mathrm{Match}(S, F) : x \mapsto F(-)x$$

is bijective for any object C and any cover $S \in J(C)$.

3.2.4 The Category of Directed Graphs as a Grothendieck Topos

Now we derive a condition in which a presheaf on $\mathcal{C}_M$ becomes J_M-sheaf. Yoneda's lemma says that $F(i) \cong \mathrm{Match}(t_i, F)$ holds by κ_{t_i} for any presheaf F on $\mathcal{C}_M$. Hence we can concern only whether

$$F(2) \cong \mathrm{Match}(S_M, F)$$

holds by κ_{S_M} for $S_M \in J_M(2)$. We have the following proposition.

Proposition 3.3 $\mathrm{Match}(S_M, F) \cong \mathrm{Hom}(M, L_E(F))$.

Proof. Let a natural transformation $\mu : S_M \to F$ be given. Components of μ are

$$\begin{aligned}
\mu_2 = \emptyset \quad &: \quad S_M(2) = \emptyset \to F(2), \\
\mu_1 \quad &: \quad S_M(1) = \{u_f | f \in M_A\} \to F(1), \\
\mu_0 \quad &: \quad S_M(0) = \{u_f m_i | f \in M_A,\ i \in \{0, 1\}\} \to F(0).
\end{aligned}$$

We define a homomorphism of directed graphs $d : M \to L_E(F)$ by

$$\begin{aligned} d_A &: M_A \to F(1) : f \mapsto \mu_1(u_f), \\ d_O &: M_O \to F(0) : n \mapsto \mu_0(u_f m_i) \text{ for } n = \partial_i^M f. \end{aligned}$$

d_O is a well-defined map by the definition of $\mathcal{C}_M$.

Conversely, suppose a homomorphism of directed graphs $d : M \to L_E(F)$ is given. A matching family $\mu : S_M \to F$ is defined by

$$\begin{aligned} \mu_1 &: S_M(1) \to F(1) : u_f \mapsto d_A(f), \\ \mu_0 &: S_M(0) \to F(0) : u_f m_i \mapsto d_O(\partial_i^M f). \end{aligned}$$

It is clear that these constructions are the inverse of each other. □

By the proposition, a necessary and sufficient condition that a presheaf F on $\mathcal{C}_M$ is a J_M-sheaf is that the map

$$\tau : F(2) \to \mathrm{Hom}(M, L_E(F)) : \alpha \mapsto d^\alpha$$

is a bijection. d^α is a homomorphism of directed graphs defined by

$$\begin{aligned} d_A^\alpha &: M_A \to F(1) : f \mapsto F(u_f)\alpha, \\ d_O^\alpha &: M_O \to F(0) : n \mapsto F(u_f m_i)\alpha \text{ for } n = \partial_i^M f. \end{aligned}$$

In other words, a presheaf F on $\mathcal{C}_M$ is J_M-sheaf if and only if

$$R_E L_E(F) \cong F$$

holds. Since $L_E R_E$ is isomorphic to the identity functor on $\mathcal{G}rph$, $R_E(G)$ is always J_M-sheaf for any directed graph G. If we denote the category of J_M-sheaves on $\mathcal{C}_M$ by $\mathcal{S}h(\mathcal{C}_M, J_M)$ then we obtain an equivalence of categories

$$\mathcal{S}h(\mathcal{C}_M, J_M) \simeq \mathcal{G}rph.$$

3.2.5 Sheafification

Given a presheaf F on $\mathcal{C}_M$, what is the best sheaf which "approximates" the presheaf F? The technique which answers this question is called *sheafification* [53]. In this subsection we calculate the sheafification of presheaves on $\mathcal{C}_M$ by a procedure so-called Grothendieck's '+'-construction.

Let F be a presheaf on a small category $\mathcal{C}$ and J a Grothendieck topology on $\mathcal{C}$. A new presheaf F^+ is defined by

$$F^+(C) = \lim_{S \in J(C)} \mathrm{Match}(S, F).$$

The colimit is taken by the reverse inclusion order defined on $J(C)$. This colimit can be described as follows. Elements of the set $F^+(C)$ are equivalence classes of matching families $\mu \in \text{Match}(S, F)$. Two matching families $\mu \in \text{Match}(S, F)$ and $\nu \in \text{Match}(T, F)$ are equivalent if and only if there exists a covering sieve $R \in J(C)$ such that $R \subseteq S \cap T$ such that $\mu|_R = \nu|_R$.

In general, F^+ is not a J-sheaf but it is known that $(F^+)^+$ is a J-sheaf. However, we shall prove that F^+ is already a J_M-sheaf for a presheaf F on $\mathcal{C}_M$ in what follows.

By Yoneda's lemma, we have

$$F^+(i) = \lim_{S \in J_M(i)} \text{Match}(S, F) \cong \text{Match}(t_i, F) \cong F(i)$$

for $i = 0, 1$. For $F^+(2)$, since $\mu|_{S_M} \in \text{Match}(S_M, F)$ for any $\mu \in \text{Match}(S_M, F)$, μ is equivalent to $\mu|_{S_M}$. Besides, because two different elements in $\text{Match}(S_M, F)$ belong to different equivalence classes,

$$F^+(2) = \lim_{S \in J_M(2)} \text{Match}(S, F) \cong \text{Match}(S_M, F) \cong \text{Hom}(M, L_E(F)).$$

This implies that $F^+ \cong R_E(L_E(F))$ which means F^+ is a J_M-sheaf. Since sheafification of a presheaf is unique up to isomorphisms, we can calculate a sheafification of presheaves on $\mathcal{C}_M$ with respect to the topology J_M by applying $R_E L_E$ to them.

3.3 Information Processing Networks

Let us recall the points in the previous section. Network motifs are coherent wholes. By defining a suitable category and a topology on it, we can address the relationships between parts and whole by sheaves.

In section 2, an object in $\mathcal{G}rph$ is considered to represent a network in nature. On the other hand, an object in $\mathcal{S}ets^{\mathcal{C}_M^{op}}$ is constructed artificially in relation to finding a motif from the outside of the network. The construction would describe the wholeness of motifs in a mathematically favorable way as an equivalence of categories, however, it does not provide any suggestion what kinds of motifs arise in networks.

In this section we focus on information processing networks such as gene transcription regulation networks or neural networks. We extract a common feature of information processing networks and integrate the feature into the setting in section 2.

3.3.1 An Internal Structure of Nodes

In information processing networks, each node in a network can be both receiver and sender of information. It processes information between reception and sending. Hence it should be considered to have an internal structure. One of the simplest candidates for the internal structure is a directed graph consisting of two different nodes and a single arrow between them. The arrow corresponds to information processing, the source of the arrow corresponds to reception of

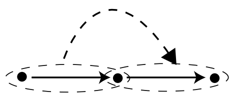

Figure 3.1: Broken ellipses denote two nodes in an information processing network. They have an internal structure that represents information processing. A broken curved arrow denotes an arrow connecting them in the network.

information and the target of the arrow corresponds to sending of information. Suppose two nodes in an information processing network are connected by an arrow. How can we describe this situation with the proposed internal structure of nodes? If we identify the sending of information at the source node with the reception of information at the target node then we could describe the situation by simply identifying the target of the arrow corresponding to the source node with the source of the arrow corresponding to the target node. The situation is depicted in Figure 3.1.

Now we integrate the above idea into Grothendieck construction in section 2. We make use of the fact that the category of directed graphs is isomorphic to a presheaf category defined by the following diagram.

$$\bullet \underset{t}{\overset{s}{\rightrightarrows}} \bullet$$

By Grothendieck construction we can give internal structures to the two nodes in the diagram. We define motif M by a directed graph

$$\bullet \overset{e_0}{\to} \bullet \overset{e_1}{\to} \bullet.$$

This motif is not a motif in the sense in section 2 but is defined by the internal structure of nodes. It represents a specific information processing pattern associated with an arrow in a network. We call the motif M here *intrinsic motif*. In order to distinguish it from so-called network motifs described in section 2, we call network motifs *extrinsic motifs* since they are found by an external observer who describes the local structure of networks. On the other hand, the intrinsic motif M is relevant to how the specific local structures of information processing networks (BF and FFL) appear as we explain bellow.

Let $\mathcal{C}_M^*$ be a finite category with two objects $1, 2$. We have just two morphisms corresponding to e_0, e_1 from 1 to 2 other than identities. The two morphisms are also denoted by e_0, e_1 since there would be no confusion. $\mathcal{C}_M^*$ is a subcategory of $\mathcal{C}_M$. We denote the restriction of the functor $E : \mathcal{C}_M \to \mathcal{G}rph$ to $\mathcal{C}_M^*$ by the same symbol E. Note that a presheaf on $\mathcal{C}_M^*$ can be seen as a directed graph $F = (F(2), F(1), F(e_0), F(e_1))$. A functor R_E from $\mathcal{G}rph$ to $\mathcal{S}ets^{\mathcal{C}_M^{*\,op}} \cong \mathcal{G}rph$ can be defined by the same way as in section 2. By Grothendieck construction, R_E has a left adjoint L_E. We just give a concrete description of the left adjoint omitting the calculation again.

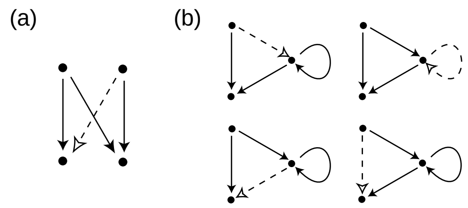

Figure 3.2: If real arrows exist then dotted arrows must exist. (a)bi-fan (BF). (b)feed-forward loop (FFL) with a loop.

Let F be a presheaf on $\mathcal{C}_M^*$. We have

$$L_E(F) = F \otimes_{\mathcal{C}_M^*} E \cong F(1) \underset{\partial_1^F}{\overset{\partial_0^F}{\rightrightarrows}} F(1) \times \{0,1\}/\sim,$$

where $\sim$ is an equivalence relation on $F(1) \times \{0,1\}$ generated by the following relation R on $F(1) \times \{0,1\}$. For $(a,1),(b,0) \in F(1) \times \{0,1\}$

$$(a,1)R(b,0) \Leftrightarrow \exists \alpha \in F(2) \text{ s.t. } a = F(e_0)\alpha, b = F(e_1)\alpha.$$

We define $\partial_i^F(a) = [(a,i)]$ $(i = 0,1)$ for $a \in F(1)$, where $[(a,i)]$ is an equivalence class that includes (a,i). The adjunction obtained here is the same one derived heuristically in chapter 2 [29].

3.3.2 A Derivation of Network Motifs

The wholeness of network motifs is represented by sheaves in section 2. However, it is not useful to consider sheaves in the setting in this section since the category $\mathcal{C}_M^*$ loses information how arrows are connected in M. Instead, we adopt the condition $R_E L_E(F) \cong F$ for representation of the wholeness. This is equivalent to the condition of sheaf in section 2. Recall that a presheaf F on $\mathcal{C}_M^*$ can be seen as a directed graph $F = (F(2), F(1), F(e_0), F(e_1))$. We now consider that presheaves on $\mathcal{C}_M^*$ represent networks in nature. Objects in $\mathcal{G}rph$ are supposed to have only auxiliary roles. Roles of the presheaf category and $\mathcal{G}rph$ are reversed from those in section 2.

A necessary and sufficient condition that a binary directed graph F satisfies $R_E L_E(F) \cong F$ is already obtained in chapter 2 [29]. If we write $a \to b$ when there exists an arrow from a to b in F then the condition can be stated as follows.

$$\text{If } a \to b \leftarrow c \to d \text{ then } a \to d.$$

This implies that if three arrows in F make a sub-pattern of bi-fan (BF) then they are indeed included in a BF (Figure 3.2 (a)). If one of four arrows in a BF is loop then the BF becomes a feed-forward loop (FFL) with a loop (Figure 3.2

(b)). Such type of FFL with loop at the relay point often is often observed in real biological networks [2]. Thus we can derive both BF and FFL as conditional statements from algebraic descriptions of wholeness and information processing.

We can interpret the appearance of bi-fan as the stabilization of intrinsic motif M. Let F be a network (or a directed graph). For nodes $x, y \in F$, $(x,1)R(y,0)$ means that there exists an arrow from x to y, $x \to y$. Suppose $a \to b \leftarrow c \to d$ in F. This implies that

$$(a,1)R(b,0),\ (c,1)R(b,0) \text{ and } (c,1)R(d,0).$$

By the construction of an equivalence relation from R,

$$(a,1)R(b,0) = (b,0)R^{-1}(c,1) = (c,1)R(d,0)$$

implies $(a,1)R(d,0)$, which means $a \to d$. We here use the reflexive law twice, the symmetric law once and the transitive law twice. The reflexive law guarantees the identity of symbol (x,i). (x,i) represents a role (e_0 or e_1) in intrinsic motif M. The symmetric law here could be seen as a kind of feedback if we interpret an arrow in a network as a transduction of information, since the symmetric law reverses the relation $(c,1)R(b,0)$ which means $c \to b$ in the network. Finally, the transitive law provides the compositions of relations R and R^{-1}, which are interpreted as propagation of information transduction and feedback. Thus by the construction of the equivalence relation from R, roles $(a,1),(b,0),(c,1)$ and $(d,0)$ in M are integrated as a whole and stabilized. Hence we would like to say that intrinsic motif M is stable in F if $R_E L_E(F) \cong F$ holds.

3.4 Conclusions

In this chapter we derive network motifs found in information processing networks in nature from purely algebraic considerations on wholeness and information processing. We assume that nodes in information processing networks have a simple internal structure. The internal structure of a node constructs an information processing pattern associated with an arrow in a network. The wholeness of the information processing pattern is materialized as network motifs such as BF and FFL.

We can generalize the idea of intrinsic motif described in this chapter. The generalization is presented in next chapter. Another example of intrinsic motif which is relevant to real networks will be found. See (14) of section 4.2.

Chapter 4

Mathematics of Intrinsic Motifs

This chapter is devoted to further mathematical aspects of ideas in chapter 2 and 3.

4.1 Grothendieck Construction on Presheaf Categories

In this section we review Grothendieck construction on presheaf categories used in the previous and present chapters [53].

Let $\mathcal{C}$ be a small category and $\mathcal{E}$ be a cocomplete category. Consider a functor E from $\mathcal{C}$ to $\mathcal{E}$. E induces a functor R_E from $\mathcal{E}$ to $\mathcal{S}ets^{\mathcal{C}^{op}}$, where $\mathcal{S}ets$ is the category of sets. R_E is defined by

$$R_E(G) = \mathrm{Hom}(E(-), G)$$

for an object G in $\mathcal{E}$. Grothendieck construction says that R_E has a left adjoint functor L_E from $\mathcal{S}ets^{\mathcal{C}^{op}}$ to $\mathcal{E}$. L_E is constructed as follows.

Let F be a presheaf on $\mathcal{C}$, that is, an object of $\mathcal{S}ets^{\mathcal{C}^{op}}$. We define the *category of elements* of F denoted by $\int_{\mathcal{C}} F$. Objects in $\int_{\mathcal{C}} F$ are all pairs (C, f) where C is an object of $\mathcal{C}$ and f is an element $f \in F(C)$. Morphisms $(C', f') \to (C, f)$ are morphisms $u : C' \to C$ in $\mathcal{C}$ such that $F(u)f = f'$. A projection functor

$$\pi_F : \int_{\mathcal{C}} F \to \mathcal{C}$$

is defined by $\pi_F(C, f) = C$. We define L_E by

$$L_E(F) = \mathrm{Colim}(\int_{\mathcal{C}} F \overset{\pi_F}{\to} \mathcal{C} \overset{E}{\to} \mathcal{E}).$$

Let us prove that L_E is indeed a left adjoint functor to R_E. In other words, we would like to show that a natural isomorphism

$$\mathrm{Hom}(L_E(F), G) \cong \mathrm{Hom}(F, R_E(G))$$

for a presheaf F on $\mathcal{C}$ and an object G of $\mathcal{E}$. Here we only show the bijection. Given a natural transformation $\mu : F \to R_E(G)$, it consists of a family $\{\mu_C\}_C$ indexed by objects C in $\mathcal{C}$. Each μ_C is a map

$$\mu_C : F(C) \to \mathrm{Hom}(E(C), G).$$

By the naturality of μ, the following diagram commutes for any morphism $u : C' \to C$.

$$\begin{array}{ccc} F(C) & \xrightarrow{\mu_C} & \mathrm{Hom}(E(C), G) \\ {\scriptstyle F(u)}\downarrow & & \downarrow{\scriptstyle (-)\circ E(u)} \\ F(C') & \xrightarrow{\mu_{C'}} & \mathrm{Hom}(E(C'), G) \end{array}$$

On the other hand, μ can be seen as a family $\{\mu_C(f) : E(C) \to G\}_{(C,f)}$ of morphisms in $\mathcal{E}$ indexed by objects (C, f) in $\int_{\mathcal{C}} F$. Then the above diagram becomes the following diagram.

$$\begin{array}{ccccc} E(C) & = & E\pi_F(C, f) & \xrightarrow{\mu_C(f)} & G \\ {\scriptstyle E(u)}\uparrow & & \uparrow & & \| \\ E(C') & = & E\pi_F(C', f') & \xrightarrow{\mu_{C'}(f')} & G \end{array}$$

One can see that the morphisms $\mu_C(f)$ form a cocone from the functor $E\pi_F$ to G. Since $L_E(F)$ is the colimit for the functor $E\pi_F$, there exists a unique morphism from $L_E(F)$ to G. Thus we obtain a bijection between $\mathrm{Hom}(L_E(F), G)$ and $\mathrm{Hom}(F, R_E(G))$.

Now consider the case $\mathcal{E} = \mathcal{S}ets^{\mathcal{D}^{op}}$ for a small category $\mathcal{D}$. Consider a presheaf F on $\mathcal{C}$ and a functor $E : \mathcal{C} \to \mathcal{S}ets^{\mathcal{D}^{op}}$. We shall see the left adjoint functor can be seen as a generalized tensor product $L_E(F) = F \otimes_{\mathcal{C}} E$. By the standard construction of colimits from coproducts and coequalizers, we have the following diagram.

$$\coprod_{u:(C',f')\to(C,f)} E(C') \underset{\eta}{\overset{\zeta}{\rightrightarrows}} \coprod_{(C,f)} E(C) \xrightarrow{\chi} F \otimes_{\mathcal{C}} E$$

On an object D of $\mathcal{D}$, the diagram becomes

$$\coprod_{C',C} F(C) \times \mathrm{Hom}(C', C) \times E(C')(D) \underset{\eta_D}{\overset{\zeta_D}{\rightrightarrows}} \coprod_{C} F(C) \times E(C)(D) \xrightarrow{\chi_D} (F \otimes_{\mathcal{C}} E)(D),$$

where

$$\zeta_D(f, u, g) = (F(u)f, g), \ \eta_D(f, u, g) = (f, E(u)_D g)$$

for $(f, u, g) \in F(C) \times \mathrm{Hom}(C', C) \times E(C')(D)$,

$$\chi_D(f, h) = f \otimes h$$

for $(f, h) \in F(C) \times E(C)(D)$ and

$$(F \otimes_{\mathcal{C}} E)(D) = \coprod_C F(C) \times E(C)(D)/\sim .$$

$\sim$ is an equivalence relation generated by $\zeta_D(f, u, g) \sim \eta_D(f, u, g)$. We denote the equivalence class which includes (f, h) by $f \otimes h$. Then we have $F(u)f \otimes g = f \otimes E(u)_D g$.

For a morphism $v : D' \to D$ in $\mathcal{D}$, we define

$$(F \otimes_{\mathcal{C}} E)(v) : (F \otimes_{\mathcal{C}} E)(D) \to (F \otimes_{\mathcal{C}} E)(D')$$

by $f \otimes h \mapsto f \otimes E(C)(v)h$ for $(f, h) \in F(C) \times E(C)(D)$. One can show that this map is well-defined. Indeed, we have $F(u)f \otimes g = f \otimes E(u)_D g$ for $f \in F(C)$, $g \in E(C')(D)$ and $u : C' \to C$. We would like to show that

$$F(u)f \otimes E(C)(v)g = f \otimes E(C)(v)E(u)_D g.$$

However, since $E(u)$ is a natural transformation, the diagram

$$\begin{tikzcd} E(C)(D) \arrow[r, "E(C)(v)"] & E(C)(D') \\ E(C')(D) \arrow[u, "E(u)_D"] \arrow[r, "E(C')(v)"] & E(C')(D') \arrow[u, "E(u)_{D'}"'] \end{tikzcd}$$

commutes. Hence we obtain

$$F(u)f \otimes E(C)(v)g = f \otimes E(u)_D E(C)(v)g = f \otimes E(C)(v)E(u)_D g.$$

Finally, we present an adjunction between two functor categories $\mathrm{Func}(\mathcal{C}, \mathcal{S}ets^{\mathcal{D}^{op}})$ and $\mathrm{Func}(\mathcal{S}ets^{\mathcal{C}^{op}}, \mathcal{S}ets^{\mathcal{D}^{op}})$, which will be used later in this chapter. Consider a function $\mathcal{F}$ which assigns each functor $A : \mathcal{C} \to \mathcal{S}ets^{\mathcal{D}^{op}}$ with a functor $L_A : \mathcal{S}ets^{\mathcal{C}^{op}} \to \mathcal{S}ets^{\mathcal{D}^{op}}$ and a function $\mathcal{G}$ which assigns each functor $L : \mathcal{S}ets^{\mathcal{C}^{op}} \to \mathcal{S}ets^{\mathcal{D}^{op}}$ with a functor $L(\mathbf{y}(-)) : \mathcal{C} \to \mathcal{S}ets^{\mathcal{D}^{op}}$, where $\mathbf{y} : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$ is the Yoneda embedding $C \mapsto \mathbf{y}(C) = \mathrm{Hom}(-, C)$. $\mathcal{F}$ and $\mathcal{G}$ can become functors in natural ways. In what follows, we prove that $\mathcal{F}$ is a left adjoint functor to $\mathcal{G}$.

Theorem 4.1 *For any functor $A : \mathcal{C} \to \mathcal{S}ets^{\mathcal{D}^{op}}$ and functor $L : \mathcal{S}ets^{\mathcal{C}^{op}} \to \mathcal{S}ets^{\mathcal{D}^{op}}$, we have a bijection*

$$\mathrm{Nat}(L_A, L) \cong \mathrm{Nat}(A, L(\mathbf{y}(-)))$$

which is natural in A and L.

Proof. We only prove the bijection. We define a function

$$\varphi : \mathrm{Nat}(L_A, L) \to \mathrm{Nat}(A, L(\mathbf{y}(-)))$$

as follows. Consider a natural transformation $\nu : L_A \to L$. Then $\varphi(\nu)$ is a natural transformation $A \to L(\mathbf{y}(-))$ with components $\varphi(\nu)_C : A(C) \to L(\mathbf{y}(C))$ for objects C in $\mathcal{C}$. Since $A(C)$ and $L(\mathbf{y}(C))$ are presheaves on $\mathcal{D}$, $\varphi(\nu)_C$ is also a natural transformation with components $\varphi(\nu)_{C,D} : A(C)(D) \to L(\mathbf{y}(C))(D)$ for objects D in $\mathcal{D}$. Hence we define

$$\varphi(\nu)_{C,D}(x) = \nu_{\mathbf{y}(C),D}(\mathrm{id}_C \otimes x)$$

for $x \in A(C)(D)$, where $\nu_{\mathbf{y}(C),D} : (\mathbf{y}(C) \otimes_{\mathcal{C}} A)(D) \to L(\mathbf{y}(C))(D)$ is a component of natural transformation ν.

On the other hand, we define a function

$$\varphi^{-1} : \mathrm{Nat}(A, L(\mathbf{y}(-))) \to \mathrm{Nat}(L_A, L)$$

, which will be revealed to be the inverse of φ, as follows. Given a natural transformation $\mu : A \to L(\mathbf{y}(-))$, a natural transformation $\varphi^{-1}(\mu) : L_A \to L$ is defined by

$$\varphi^{-1}(\mu)_{F,D}(f \otimes x) = L(F(-)f)_D(\mu_{C,D}(x))$$

for $f \in F(C)$ and $x \in A(C)(D)$. Note that $\varphi^{-1}(\mu)$ consists of components $\varphi^{-1}(\mu)_F : F \otimes_{\mathcal{C}} A \to L(F)$ for presheaves F on $\mathcal{C}$ and $\varphi^{-1}(\mu)_F$, which is also a natural transformation, consists of components $\varphi^{-1}(\mu)_{F,D} : (F \otimes_{\mathcal{C}} A)(D) \to L(F)(D)$ for objects D in $\mathcal{D}$. $F(-)f : \mathbf{y}(C) \to F$ is a natural transformation with components $(F(-)f)_{C'} : \mathrm{Hom}(C', C) \to F(C) : u \mapsto F(u)f$. Thus $L(F(-)f) : L(\mathbf{y}(C)) \to L(F)$ is a natural transformation with components $L(F(-)f)_D : L(\mathbf{y}(C))(D) \to L(F)(D)$. Let us check $\varphi^{-1}(\mu)_{F,D}$ is indeed a well-defined map. Given a morphism $u : C' \to C$ in $\mathcal{C}$ and elements $f \in F(C)$, $x \in A(C')(D)$, we have $f \otimes A(u)_D x = F(u)f \otimes x$ by the definition of tensor product. It suffices to show that

$$L(F(-)f)_D(\mu_{C,D}(A(u)_D x)) = L(F(-)F(u)f)_D(\mu_{C',D}(x)).$$

However, since μ is a natural transformation, the diagram

$$\begin{array}{ccc} A(C)(D) & \xrightarrow{\mu_{C,D}} & L(\mathbf{y}(C))(D) \\ {\scriptstyle A(u)_D}\Big\uparrow & & \Big\uparrow{\scriptstyle L(\mathbf{y}(u))_D} \\ A(C')(D) & \xrightarrow{\mu_{C',D}} & L(\mathbf{y}(C'))(D) \end{array}$$

commutes. Therefore

$$\begin{aligned} L(F(-)f)_D(\mu_{C,D}(A(u)_D x)) &= L(F(-)f)_D(L(\mathbf{y}(u))_D(\mu_{C',D}(x))) \\ &= L(F(-)f \circ \mathbf{y}(u))_D(\mu_{C',D}(x)) \\ &= L(F(u \circ (-))f)_D(\mu_{C',D}(x)) \\ &= L(F(-)F(u)f)_D(\mu_{C',D}(x)). \end{aligned}$$

Now we prove $\varphi \circ \varphi^{-1} = \mathrm{id}_{\mathrm{Nat}(A, L(\mathbf{y}(-)))}$ and $\varphi^{-1} \circ \varphi = \mathrm{id}_{\mathrm{Nat}(L_A, L)}$. Given a natural transformation $\mu : A \to L(\mathbf{y}(-))$,

$$\begin{aligned}
\varphi(\varphi^{-1}(\mu))_{C,D}(x) &= \varphi^{-1}(\mu)_{\mathbf{y}(C),D}(\mathrm{id}_C \otimes x) \\
&= L(\mathbf{y}(C)(-)\mathrm{id}_C)_D(\mu_{C,D}(x)) \\
&= L(\mathrm{id}_{\mathbf{y}(C)})_D(\mu_{C,D}(x)) \\
&= \mathrm{id}_{L(\mathbf{y}(C)),D}(\mu_{C,D}(x)) = \mu_{C,D}(x)
\end{aligned}$$

for $x \in A(C)(D)$. Thus we obtain $\varphi \circ \varphi^{-1}(\mu) = \mu$.

On the other hand, for $f \in F(C)$ and $x \in A(C)(D)$,

$$\begin{aligned}
\varphi^{-1}(\varphi(\nu))_{F,D}(f \otimes x) &= L(F(-)f)_D(\varphi(\nu)_{C,D}(x)) \\
&= L(F(-)f)_D(\nu_{\mathbf{y}(C),D}(\mathrm{id}_C \otimes x)).
\end{aligned}$$

Since ν is a natural transformation, the following diagram commutes.

$$\begin{tikzcd}
L_A(F)(D) \arrow[r, "\nu_{F,D}"] & L(F)(D) \\
L_A(\mathbf{y}(C))(D) \arrow[u, "L_A(F(-)f)_D"] \arrow[r, "\nu_{\mathbf{y}(C),D}"] & L(\mathbf{y}(C))(D) \arrow[u, "L(F(-)f)_D"']
\end{tikzcd}$$

Thus

$$\begin{aligned}
L(F(-)f)_D(\nu_{\mathbf{y}(C),D}(\mathrm{id}_C \otimes x)) &= \nu_{F,D}(L_A(F(-)f)_D(\mathrm{id}_C \otimes x)) \\
&= \nu_{F,D}(F(\mathrm{id}_C)f \otimes x) = \nu_{F,D}(f \otimes x).
\end{aligned}$$

This shows $\varphi^{-1} \circ \varphi = \mathrm{id}_{\mathrm{Nat}(L_A, L)}$. □

4.2 Generalized Intrinsic Motifs

In this section we consider a generalization of the idea of intrinsic motif in the previous chapter. We consider the same internal structure of nodes as in the previous chapter, which consists of two distinct nodes and a single arrow between them. In the previous chapter, this structure is interpreted as a pattern of information processing. If two nodes are connected by an arrow then corresponding internal structures of the nodes are connected in a serial manner. In this section we extend how two internal structures are connected.

Let $M = (M_A, M_O, \partial_0^M, \partial_1^M)$ be a directed graph. As in the previous chapter, we assume that for any $x \in M_O$ there exists $f \in M_A$ such that $\partial_0^M f = x$ or $\partial_1^M f = x$. M is regarded as a generalized intrinsic motif in what follows.

Let $\mathcal{C}_M^*$ is a category with two objects $1, 2$ and morphisms

$$1 \xrightarrow{u_f} 2$$

for each $f \in M_A$ in addition to the identities. Note that $\mathcal{C}_M^*$ is determined by the number of arrows in M. We restrict the functor $E : \mathcal{C}_M \to \mathcal{G}rph$ in the previous section to $\mathcal{C}_M^*$ and again denote it by E. A functor R_E from $\mathcal{G}rph$ to $\mathcal{S}ets^{\mathcal{C}_M^{*\,op}}$ is defined by

$$R_E(G) = \mathrm{Hom}(E(-), G)$$

for a directed graph G.

By Grothendieck construction, a tensor product functor L_E that is a left adjoint to R_E is defined. Let F be a presheaf on $\mathcal{C}_M^*$. Then we have

$$L_E(F) = F \otimes_{\mathcal{C}_M^*} E \cong F(1) \overset{\partial_0^F}{\underset{\partial_1^F}{\rightrightarrows}} F(1) \times \{0,1\}/\sim .$$

$\sim$ is an equivalence relation on $F(1) \times \{0,1\}$ generated by the following relation R.

$$(a,i)R(b,j) \Leftrightarrow \exists \alpha \in F(2)\ \exists f,g \in M_A \text{ s.t. } a = F(u_f)\alpha, b = F(u_g)\alpha, \partial_i^M f = \partial_j^M g$$

for $(a,i),(b,j) \in F(1) \times \{0,1\}$. We define

$$\partial_i^F(a) = [(a,i)]$$

for $a \in F(1)$, where $[(a,i)]$ is an equivalence class that includes (a,i).

Here we prove that L_E is a left adjoint functor to R_E directly instead of calculating the tensor product.

Theorem 4.2 *We have a natural isomorphism*

$$\mathcal{G}rph(L_E(F), G) \cong \mathcal{S}ets^{\mathcal{C}_M^{*\,op}}(F, R_E(G))$$

for any directed graph $G = (A, O, \partial_0, \partial_1)$ *and any presheaf on* $\mathcal{C}_M^*$.

Proof. We only describe the construction of isomorphism.

$$\varphi : \mathcal{G}rph(L_E(F), G) \to \mathcal{S}ets^{\mathcal{C}_M^{*\,op}}(F, R_E(G))$$

is defined as follows. Given a homomorphism of directed graphs $d : L_E(F) \to G$, we have two maps

$$\begin{aligned} d_O &: F(1) \times \{0,1\}/\sim \to O, \\ d_A &: F(1) \to A. \end{aligned}$$

We would like to define components of natural transformation $\varphi(d)$ from F to $R_E(G)$

$$\begin{aligned} \varphi(d)_1 &: F(1) \to R_E(G)(1) = \mathrm{Hom}(\{n_0 \to n_1\}, G), \\ \varphi(d)_2 &: F(2) \to R_E(G)(2) = \mathrm{Hom}(M, G). \end{aligned}$$

For $a \in F(1)$, $\varphi(d)_1(a)$ is defined by a homomorphism of directed graphs determined by $(\varphi(d)_1(a))_A(\to) = d_A(a)$. For $\alpha \in F(2)$, $\varphi(d)_2(\alpha)$ is defined by a homomorphism of directed graphs determined by $(\varphi(d)_2(\alpha))_A(f) = d_A(F(u_f)\alpha)$ for any $f \in M_A$.

The inverse of φ

$$\varphi^{-1} : \mathcal{S}ets^{\mathcal{C}_M^{*\,op}}(F, R_E(G)) \to \mathcal{G}rph(L_E(F), G)$$

is defined as follows.

Let $\mu : F \to R_E(G)$ be given. We would like to define a homomorphism of directed graphs $\varphi^{-1}(\mu) : L_E(F) \to G$ from

$$\mu_1 : F(1) \to \mathrm{Hom}(\{n_0 \to n_1\}, G),$$
$$\mu_2 : F(2) \to \mathrm{Hom}(M, G).$$

We define

$$\varphi^{-1}(\mu)_A : F(1) \to A$$

by $\varphi^{-1}(\mu)_A(a) = \mu_1(a)_A(\to)$ for $a \in F(1)$.

$$\varphi^{-1}(\mu)_O : F(1) \times \{0,1\}/\sim \to O$$

is defined by a map sending each $[(a,i)]$ to $\partial_i \mu_1(a)_A(\to)$. This map is well-defined. In order to check this, it is sufficient to prove that if $(a,i)R(b,j)$ then $\partial_i\mu_1(a)_A(\to) = \partial_j\mu_1(b)_A(\to)$. If $(a,i)R(b,j)$ then

$$\exists \alpha \in F(2)\ \exists f, g \in M_A \text{ s.t. } a = F(u_f)\alpha, b = F(u_g)\alpha, \partial_i^M f = \partial_j^M g.$$

Hence we have

$$\begin{aligned}
\partial_i\mu_1(a)_A(\to) &= \partial_i\mu_1(F(u_f)\alpha)_A(\to) = \partial_i(\mu_2(\alpha)E(u_f))_A(\to) \\
&= \partial_i\mu_2(\alpha)_A(E(u_f)_A(\to)) = \partial_i\mu_2(\alpha)_A(f) \\
&= \mu_2(\alpha)_O\partial_i^M(f) = \mu_2(\alpha)_O\partial_j^M(g) \\
&= \partial_j\mu_2(\alpha)_A(g) = \partial_j\mu_2(\alpha)_A(E(u_g)_A(\to)) \\
&= \partial_j\mu_1(F(u_g)\alpha)_A(\to) = \partial_j\mu_1(b)_A(\to).
\end{aligned}$$

□

Let us denote the restriction of Grothendieck topology J_M on $\mathcal{C}_M$ to $\mathcal{C}_M^*$ by again J_M. The unique non-maximal covering sieve is $S_M = \{u_f\}_{f \in M_A} \in J_M(2)$. J_M is indeed a Grothendieck topology on $\mathcal{C}_M^*$, however, it seems that it is not useful to consider the condition of J_M-sheaf for presheaves on $\mathcal{C}_M^*$. This is because the structure of $\mathcal{C}_M^*$ is only dependent on the number of arrows in M. There is no information how the arrows in M are related with each other. For example, the construction of the isomorphism $\mathrm{Match}(S_M, F) \cong \mathrm{Hom}(M, L_E(F))$, which is important in the former half of the previous section does not hold. Indeed, consider $\mu : S_M \to F$. Components of μ are

$$\begin{aligned}
\mu_2 = \emptyset &: S_M(2) = \emptyset \to F(2), \\
\mu_1 &: S_M(1) = \{u_f | f \in M_A\} \to F(1).
\end{aligned}$$

μ_1 can be any map from $S_M(1)$ to F(1). Let us define a homomorphism of directed graphs $d : M \to L_E(F)$ by

$$d_A \quad : \quad M_A \to F(1) : f \mapsto \mu_1(u_f)$$

as in proposition 3.3.

In order d to be a homomorphism of directed graphs, it must satisfy $d_O \partial_i^M f = \partial_i^F d_A f$. Hence d_O must be defined by

$$d_O \quad : \quad M_O \to F(0) : n \mapsto [(\mu_1(u_f), i)] \text{ for } n = \partial_i^M f.$$

However, d_O is not a well-defined map in general. Suppose $n = \partial_i^M f = \partial_j^M g$. In order d_O to be a well-defined map, $[(\mu_1(u_f), i)] = [(\mu_1(u_g), j)]$ must hold. However, since μ_1 is arbitrary map, there is no α such that $\mu_1(u_f) = F(u_f)\alpha, \mu_1(u_g) = F(u_g)\alpha$ in general.

Thus $\mathrm{Match}(S_M, F) \cong \mathrm{Hom}(M, L_E(F))$ does not hold in general, however, we can consider a map

$$\tau : F(2) \to \mathrm{Hom}(M, L_E(F)).$$

τ sends each $\alpha \in F(2)$ to a homomorphism of directed graphs d^α defined by

$$\begin{aligned} d_A^\alpha \quad &: \quad M_A \to F(1) : f \mapsto F(u_f)\alpha, \\ d_O^\alpha \quad &: \quad M_O \to (F(1) \times \{0, 1\})/\sim : n \mapsto [(F(u_f)\alpha, i)] \text{ for } n = \partial_i^M f. \end{aligned}$$

As in the previous section, τ is a bijection if and only if

$$F \cong R_E L_E(F)$$

holds by $\eta_F : F \to R_E L_E(F)$, which is a component of the unit η of the adjunction.

This motivates us to adopt the bijectivity of τ as a representation of wholeness rather than sheaf as mentioned briefly in the latter half of the previous section.

Next we consider the case in which M has just two arrows. In this case, $\mathcal{S}ets^{\mathcal{C}_M^{*\,op}}$ is isomorphic to $\mathcal{G}rph$. There are finite possibilities for M. We determine for which F τ becomes bijection for each case.

By the definition of τ we have the following proposition.

Proposition 4.3 *τ is injective if and only if*

$$F(u_f)\alpha = F(u_f)\beta \text{ for } \forall f \in M_A \Rightarrow \alpha = \beta.$$

We denote the two arrows in M by $\{e_0, e_1\}$. $F(u_{e_0})$ is the source map for F and $F(u_{e_1})$ is the target map for F. That is,

$$F(2) \underset{F(u_{e_0})}{\overset{F(u_{e_1})}{\rightrightarrows}} F(1)$$

is a directed graph $(F(2), F(1), F(u_{e_0}), F(u_{e_1}))$. For simplicity, we denote $F(u_{e_i})$ by $F(e_i)$. Thus proposition 4.3 means that there is at most one arrow for any ordered pair of nodes. In other words, F is a binary directed graph.

In order to obtain a necessary and sufficient condition for surjectivity of τ, we prepare the following lemma.

Lemma 4.4 *There is a one-to-one correspondence between homomorphisms of directed graphs $d : M \to L_E(F)$ and ordered pairs $(a_0, a_1) \in F(1) \times F(1)$ such that*

$$\partial_i^M e_k = \partial_j^M e_l \Rightarrow (a_k, i) \sim (a_l, j).$$

Proof. Given a homomorphism of directed graph $d : M \to L_E(F)$, if $\partial_i^M e_k = \partial_j^M e_l$ then

$$[(d_A(e_k), i)] = \partial_i^F d_A(e_k) = d_O(\partial_i^M e_k) = d_O(\partial_j^M e_l) = \partial_j^F d_A(e_l) = [(d_A(e_l), j)].$$

Thus $(d_A(e_0), d_A(e_1))$ is a pair that satisfies the condition. On the other hand, suppose $(a_0, a_1) \in F(1) \times F(1)$ that satisfies the condition is given. Let us define a map

$$d_A : M_A \to F(1)$$

by $d_A(e_0) = a_0, d_A(e_1) = a_1$. We also define a map

$$d_O : M_O \to (F(1) \times \{0, 1\})/\sim$$

by $d_O(n) = [(a_k, i)]$ for $n = \partial_i^M e_k$. This is well-defined by the condition. Furthermore, since we have $d_O(\partial_i^M e_k) = [(a_k, i)] = \partial_i^F d_A(e_k)$, $d = (d_A, d_O)$ is a homomorphism of directed graphs.

$\square$

From the lemma, a necessary and sufficient condition that τ is a surjection is

($\diamond$) For any $(a_0, a_1) \in F(1) \times F(1)$ such that $\partial_i^M e_k = \partial_j^M e_l \Rightarrow (a_k, i) \sim (a_l, j)$, there exists $\alpha \in F(2)$ such that $a_i = F(e_i)\alpha$ $(i = 0, 1)$.

In what follows, we rewrite the condition $\diamond$ to more concrete forms dependent on the combinations of conditions $\partial_i^M e_k = \partial_j^M e_l$.

There are 15 patterns for $\partial_i^M e_k = \partial_j^M e_l$. For $\partial_0^M e_0, \partial_1^M e_0, \partial_0^M e_1, \partial_1^M e_1$, there are

(i) one case in which all of them are different from each other,

$$(1) \quad \bullet \xrightarrow{e_0} \bullet \quad \bullet \xrightarrow{e_1} \bullet$$

(ii) six cases in which two of the four are the same,

$$
(2)\quad \overset{\circlearrowleft^{e_0}}{\bullet} \quad \bullet \xrightarrow{e_1} \bullet \qquad (3)\quad \bullet \xleftarrow{e_0} \bullet \xrightarrow{e_1} \bullet \qquad (4)\quad \bullet \xleftarrow{e_0} \bullet \xleftarrow{e_1} \bullet
$$

$$
(5)\quad \bullet \xrightarrow{e_0} \bullet \xrightarrow{e_1} \bullet \qquad (6)\quad \bullet \xrightarrow{e_0} \bullet \xleftarrow{e_1} \bullet \qquad (7)\quad \bullet \xrightarrow{e_0} \bullet \quad \overset{\circlearrowleft^{e_1}}{\bullet}
$$

(iii) four cases in which three of the four are the same,

$$
(8)\quad \overset{\circlearrowleft^{e_0}}{\bullet} \xrightarrow{e_1} \bullet \qquad (9)\quad \overset{\circlearrowleft^{e_0}}{\bullet} \xleftarrow{e_1} \bullet
$$

$$
(10)\quad \bullet \xleftarrow{e_0} \overset{\circlearrowleft^{e_1}}{\bullet} \qquad (11)\quad \bullet \xrightarrow{e_0} \overset{\circlearrowleft^{e_1}}{\bullet}
$$

(iv) three cases in which the four are divided into two groups with two members and all members in each group are the same,

$$
(12)\quad \overset{\circlearrowleft^{e_0}}{\bullet} \quad \overset{\circlearrowleft^{e_1}}{\bullet} \qquad (13)\quad \bullet \underset{e_1}{\overset{e_0}{\rightrightarrows}} \bullet \qquad (14)\quad \bullet \underset{e_1}{\overset{e_0}{\rightleftarrows}} \bullet
$$

(v) one case in which all the four are the same.

$$
(15)\quad {}^{e_0}\circlearrowright \bullet \circlearrowleft^{e_1}
$$

(1) τ is surjective if and only if there exists $\alpha \in F(2)$ such that $a_i = F(e_i)\alpha$ $(i = 0, 1)$ for any pair $(a_0, a_1) \in F(1) \times F(1)$. That is, there exists at least one arrow between any ordered pair of nodes in a directed graph $F = (F(2), F(1), F(e_0), F(e_1))$. Hence τ is bijective if and only if

(c1) F is a complete directed graph.

(2) The condition is just $\partial_0^M e_0 = \partial_1^M e_0$. Hence $(\diamond)$ is equivalent to the condition that $a \to b$ holds for any $(a, b) \in F(1) \times F(1)$ such that $(a, 0) \sim (a, 1)$, where we write $a \to b$ if there exists $\alpha \in F(2)$ such that $F(e_0)\alpha = a, F(e_1)\alpha = b$ for $a, b \in F(1)$. In addition, we write $a \to$ if there exists $\alpha \in F(2)$ such that $F(e_0)\alpha = a$ for $a \in F(1)$ and write $\to a$ if there exists $\alpha \in F(2)$ such that $F(e_1)\alpha = a$ for $a \in F(1)$.

We now prove that τ is surjective if and only if the following condition is satisfied.

(c2) For any $a \in F(1)$ if $a \to$ then $a \to b$ for any $b \in F(1)$.

If $(a, 0)R(b, 1)$ then

$$
\exists \beta \in F(2)\ \exists f, g \in M_A \text{ s.t. } a = F(u_f)\beta, b = F(u_g)\beta, \partial_0^M f = \partial_1^M g.
$$

Since $\partial_0^M f = \partial_1^M g$ holds, we have $f = g = e_0$. Hence $a = F(e_0)\beta = b$ and in particular, $a \to$. From this we can show that

$$
(a, 0) \sim (a, 1) \Leftrightarrow (a, 0)R(a, 1).
$$

Indeed, if $(a,0)\sim(a,1)$ then

$$(a,0)=(a_0,i_0)R(a_1,i_1)R\cdots R(a_n,i_n)=(a,1)$$

with $a_0=a_1=\cdots=a_n$. Thus we obtain $(a,0)R(a,1)$. The converse is obvious.

Now suppose that (c2) is satisfied. Consider $(a,b)\in F(1)\times F(1)$ such that $(a,0)\sim(a,1)$. By using (c2), we have $a\to b$ since $(a,0)R(a,1)$ and in particular, $a\to$. Conversely, suppose $(\diamond)$ holds. If $a\to$ then we have $(a,0)R(a,1)$. Therefore $a\to b$ for any $b\in F(1)$ by $(\diamond)$.

(3) The condition is $\partial_0^M e_0=\partial_0^M e_1$. Hence $(\diamond)$ is equivalent to the condition that $a\to b$ holds for any $(a,b)\in F(1)\times F(1)$ such that $(a,0)\sim(b,0)$. If $(a,0)R(b,0)$ then

$$\exists\beta\in F(2)\ \exists f,g\in M_A \text{ s.t. } a=F(u_f)\beta, b=F(u_g)\beta, \partial_0^M f=\partial_0^M g.$$

If $f=e_0, g=e_1$ then $a\to b$ and if $f=e_1, g=e_0$ then $b\to a$.

Therefore, if we write $a\leftrightharpoons b$ when $a\to b$ or $b\to a$ then $(\diamond)$ is equivalent to the following (c3):

(c3) If $a=c_0\leftrightharpoons c_1\leftrightharpoons\cdots\leftrightharpoons c_n=b$ for some $n\geq 0$ then $a\to b$.

This is equivalent to say that a directed graph is a graph of an equivalence relation.

(4) The condition is $\partial_0^M e_0=\partial_1^M e_1$. $(\diamond)$ is equivalent to the statement that if $(a,0)\sim(b,1)$ then $a\to b$. Since $(a,0)R(b,1)$ is

$$\exists\beta\in F(2)\ \exists f,g\in M_A \text{ s.t. } a=F(u_f)\beta, b=F(u_g)\beta, \partial_0^M f=\partial_1^M g$$

, $f=e_0, g=e_1$. Hence $(a,0)R(b,1)$ is equivalent to $a\to b$. Thus $(\diamond)$ is equivalent to the following (c4):

(c4) If $a=c_0\to c_1\leftarrow c_2\to\cdots\leftarrow c_{n-1}\to c_n=b$ for some odd number $n\geq 1$ then $a\to b$.

Moreover, by mathematical induction, (c4) can be reduced to the case $n=3$, the following (c4'):

(c4') If $a\to c_1\leftarrow c_2\to b$ then $a\to b$.

(5) The condition is $\partial_1^M e_0=\partial_0^M e_1$. Hence $(\diamond)$ is equivalent to the statement that if $(a,1)\sim(b,0)$ then $a\to b$. In this case we have $(a,1)R(b,0)\Leftrightarrow a\to b$, which is the same situation in (4), therefore a necessary and sufficient condition for $(\diamond)$ is (c4'). This case has been already appeared in the previous section as an intrinsic motif that is relevant to information processing in biological networks.

(6) $(\diamond)$ is equivalent to (c3) by the same argument in (3).

(7) This is dual of (2) (exchanging e_0 and e_1). ($\diamond$) is equivalent to the following (c7):

(c7) For any $b \in F(1)$, if $\rightarrow b$ then $a \rightarrow b$ for $a \in F(1)$.

(8) The condition consists of three equations, $\partial_0^M e_0 = \partial_1^M e_0, \partial_1^M e_0 = \partial_0^M e_1$ and $\partial_0^M e_0 = \partial_0^M e_1$.

Therefore ($\diamond$) is equivalent to the statement that if $(a,0) \sim (a,1), (a,1) \sim (b,0), (a,0) \sim (b,0)$ then $a \rightarrow b$. By the same argument as above we have

$$(a,0)R(a,1) \Leftrightarrow a \rightarrow,\ (a,1)R(b,0) \Leftrightarrow a \rightarrow b,\ (a,0)R(b,0) \Leftrightarrow a \leftrightharpoons b.$$

Let us prove that ($\diamond$) is equivalent to the following (c8):

(c8) If $\leftarrow a = c_0 \leftrightharpoons c_1 \leftrightharpoons \cdots \leftrightharpoons c_n = b$ for some $n \geq 0$ then $a \rightarrow b$.

Suppose (c8) holds. Moreover, suppose that $(a,0) \sim (a,1), (a,1) \sim (b,0)$ and $(a,0) \sim (b,0)$. Since $(a,1) \sim (b,0)$, we have

$$(a,1) = (d_0, j_0)R(d_1, j_1)R \cdots R(d_m, j_m) = (b,0).$$

There are two possibilities. First $d_0 = d_1$ and $\leftarrow a$ holds. Second $a \rightarrow d_1$. In both case, we have $\leftarrow a$. Moreover, if $(a,0) \sim (b,0)$ then we have $a = c_0 \leftrightharpoons c_1 \leftrightharpoons \cdots \leftrightharpoons c_n = b$. Hence we obtain $a \rightarrow b$ by using (c8).

Conversely, suppose ($\diamond$) holds. We also assume $\leftarrow a = c_0 \leftrightharpoons c_1 \leftrightharpoons \cdots \leftrightharpoons c_n = b$. $(a,0) \sim (a,1)$ holds by $\leftarrow a$. $(a,0) \sim (b,0)$ holds by $a = c_0 \leftrightharpoons c_1 \leftrightharpoons \cdots \leftrightharpoons c_n = b$. Since $(a,1) \sim (a,0) \sim (b,0)$, we have $(a,1) \sim (b,0)$ by the transitivity of $\sim$. Using ($\diamond$), we obtain $a \rightarrow b$.

(9) One can see ($\diamond$) is equivalent to (c8) by the same argument in (8).

(10) This is dual of (8) and ($\diamond$) is equivalent to the following condition (c10):

(c10) If $a = c_0 \leftrightharpoons c_1 \leftrightharpoons \cdots \leftrightharpoons c_n = b \leftarrow$ for some $n \geq 0$ then $a \rightarrow b$.

(11) This case is the same as (10).

(12) The condition consists of two equations $\partial_0^M e_0 = \partial_1^M e_0$ and $\partial_0^M e_1 = \partial_1^M e_1$. ($\diamond$) is equivalent to the statement that if $(a,0) \sim (a,1), (b,0) \sim (b,1)$ then $a \rightarrow b$. $(a,0)R(b,1)$ is

$$\exists \beta \in F(2)\ \exists f, g \in M_A \text{ s.t. } a = F(u_f)\beta, b = F(u_g)\beta, \partial_0^M f = \partial_1^M g$$

with $f = e_0 = g$ or $f = e_1 = g$. In both cases we have $a = b$. In the former case we have $a \rightarrow$ and the latter case we have $\rightarrow a$. If $(a,0) \sim (a,1)$ then

$$(a,0) = (c_0, i_0)R(c_1, i_1)R \cdots R(c_n, i_n) = (a,1).$$

Since $a = c_0 = c_1 = \cdots = c_n$, $(a,0) \sim (a,1)$ is equivalent to $(a,0)R(a,1)$. Therefore ($\diamond$) is equivalent to the following (c12):

(c12) If ($a \to$ or $a \leftarrow$) and ($b \to$ or $b \leftarrow$) then $a \to b$.

(13) The condition consists of two equations $\partial_0^M e_0 = \partial_0^M e_1$ and $\partial_1^M e_0 = \partial_1^M e_1$. Since $(a,i)R(b,i) \Leftrightarrow a \leftrightharpoons b$ $(i = 0,1)$, $(\diamond)$ is equivalent to (c3).

(14) The condition consists of two equations $\partial_1^M e_0 = \partial_0^M e_1$ and $\partial_1^M e_1 = \partial_0^M e_0$. $(\diamond)$ becomes the statement that if $(a,1) \sim (b,0), (a,0) \sim (b,1)$ then $a \to b$. $(a,1)R(b,0)$ is

$$\exists \beta \in F(2)\ \exists f,g \in M_A \text{ s.t. } a = F(u_f)\beta, b = F(u_g)\beta, \partial_1^M f = \partial_0^M g$$

with $f = e_0, g = e_1$ or $f = e_1, g = e_0$. In the former, $a \to b$ and the latter $b \to a$. Therefore $(\diamond)$ is equivalent to the following (c14):

(c14) If $a = c_0 \leftrightharpoons c_1 \leftrightharpoons \cdots \leftrightharpoons c_n = b$ for some odd number $n \geq 1$ then $a \to b$.

This condition is equivalent to the following (c14').

(c14') (i) If $a \to b$ then $b \to a$, that is, F is a symmetric directed graph.
(ii) If $a \to b \to c \to d$ then $a \to d$.

If (c14) holds then we obtain (c14') by considering $n = 1$ and $n = 3$ in (c14). The converse is mathematical induction. (c14) with $n = 1$ holds by (i) of (c14'). Suppose (c14) with $n = 2k-1$ holds $(k \geq 1)$. If we have

$$c_0 \leftrightharpoons c_1 \leftrightharpoons \cdots \leftrightharpoons c_{2k-1} \leftrightharpoons c_{2k} \leftrightharpoons c_{2k+1}$$

then by the assumption of induction $c_0 \to c_{2k-1}$. By (i) of (c14') we can assume that

$$c_0 \to c_{2k-1} \to c_{2k} \to c_{2k+1}.$$

By (ii) of (c14') we obtain $c_0 \to c_{2k+1}$. Thus (c14) with $n = 2k+1$ holds.

Now we could expect that if a symmetric network has an intrinsic motif of type (14) then the square pattern is an extrinsic motif (or a network motif). Indeed, protein-protein networks have the square pattern as a network motif [117]. They would have intrinsic motif (14) since an interaction between two proteins is represented by the bi-directional way in [117].

(15) All equations are included. Both $(a,i)R(b,i)(i = 0,1)$ and $(a,1)R(b,0)$ are equivalent to the following condition.

$$a \leftrightharpoons b \text{ if } a \neq b,$$
$$a \leftrightharpoons \text{ if } a = b.$$

Hence $(\diamond)$ is equivalent to the following condition (c15).

(c15) If $\leftrightharpoons a = c_0 \leftrightharpoons c_1 \leftrightharpoons \cdots \leftrightharpoons c_n = b \leftrightharpoons$ for some $n \geq 0$ then $a \to b$.

Thus we can classify the fifteen intrinsic motifs into ten conditions (c1), (c2), (c3), (c4), (c7), (c8), (c10), (c12), (c14) and (c15).

4.3 Further Generalization

In this section we further generalize the construction in the previous section. Let $\mathcal{C}$ be a category generated by the following diagram with no relation.

$$1 \underset{m_1}{\overset{m_0}{\rightrightarrows}} 2$$

We consider a functor $M : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$. We identify $\mathcal{S}ets^{\mathcal{C}^{op}}$ with the category of directed graphs $\mathcal{G}rph$. In particular, we regard $M(i)$ as a directed graph

$$\begin{aligned} M(i) &= (M(i)_A, M(i)_O, \partial_0^{M(i)}, \partial_1^{M(i)}) \\ &:= (M(i)(2), M(i)(1), M(i)(m_0), M(i)(m_1)) \end{aligned}$$

for $i = 0, 1$.

This functor induces an adjunction

$$\mathcal{S}ets^{\mathcal{C}^{op}} \underset{R_M}{\overset{L_M}{\rightleftarrows}} \mathcal{S}ets^{\mathcal{C}^{op}}$$

as we have seen in section 1 of this chapter.

In the previous section we always have $M(1) = \{n_1 \to n_2\}$. In this section we eliminate this constraint. However, instead of this, we assume that

$$M(2)_A \subseteq M(m_0)_A(M(1)_A) \cup M(m_1)_A(M(1)_A)$$

and

$$M(2)_O \subseteq M(m_0)_O(M(1)_O) \cup M(m_1)_O(M(1)_O),$$

which are satisfied by intrinsic motifs in the previous section. We also call functors $M : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$ that satisfy the above condition *intrinsic motifs*. Unfortunately, this assumption excludes a trivial case

$$M(1) = \{*\},\ M(2) = \{n_1 \to n_2\}$$

with $M(m_i)_O(*) = n_i$ $(i = 0, 1)$, which provides the identity functor by Grothendieck construction (that is, both R_M and L_M are the identity functor on $\mathcal{S}ets^{\mathcal{C}^{op}}$), however, this assumption makes calculations of tensor products much easier.

Now let us calculate a concrete representation of the tensor product between a presheaf F on $\mathcal{C}$ and an intrinsic motif M. By the calculation in section 1 of this chapter, we have

$$(F \otimes_{\mathcal{C}} M)_A = (F \otimes_{\mathcal{C}} M)(2) = ((F(1) \times M(1)_A) \coprod (F(2) \times M(2)_A))/\sim_2$$

and

$$(F \otimes_{\mathcal{C}} M)_O = (F \otimes_{\mathcal{C}} M)(1) = ((F(1) \times M(1)_O) \coprod (F(2) \times M(2)_O))/\sim_1,$$

where $\sim_2$ is an equivalence relation generated by the relation R_2 defined by

$$(F(m_i)\alpha, f)R_2(\alpha, M(m_i)_A f)$$

for $\alpha \in F(2),\ f \in M(1)_A$ and $i = 0, 1$. $\sim_1$ is an equivalence relation generated by the relation R_1 defined by

$$(F(m_i)\alpha, n)R_1(\alpha, M(m_i)_O n)$$

for $\alpha \in F(2),\ n \in M(1)_O$ and $i = 0, 1$.

For any $(\alpha, g) \in F(2) \times M(2)_A$, there exists $i \in \{0, 1\}$ and an arrow $f \in M(1)_A$ such that $g = M(m_i)_A f$, since we assume that

$$M(2)_A \subseteq M(m_0)_A(M(1)_A) \cup M(m_1)_A(M(1)_A).$$

Hence we have $(\alpha, g) = (\alpha, M(m_i)_A f)R_2(F(m_i)\alpha, f)$. Thus for any $(\alpha, g) \in F(2) \times M(2)_A$ there exists $(x, f) \in F(1) \times M(1)_A$ such that $(\alpha, g) \sim_2 (x, f)$. On the other hand, for $(x, f), (y, g) \in F(1) \times M(1)_A$, suppose that $x = F(m_{j_0})\alpha$ and $y = F(m_{j_1})\beta$ for some $\alpha, \beta \in F(2)$. If $(x, f)R_2^{-1}(\gamma, h)R_2(y, g)$ for some $(\gamma, h) \in F(2) \times M(2)_A$ then $\alpha = \gamma = \beta$ and $M(m_{j_0})_A f = M(m_{j_1})_A g$ since $(\alpha, M(m_{j_0})_A f)R_2(F(m_{j_0})\alpha, f)$ and $(\beta, M(m_{j_1})_A g)R_2(F(m_{j_1})\beta, g)$. Thus if we define a relation R'_2 on $F(1) \times M(1)_A$ by

$$\begin{aligned}(x, f)R'_2(y, g) \quad \Leftrightarrow \quad & \exists \alpha \in F(2)\ \exists j_0, j_1 \in \{0, 1\} \\ \text{s.t.} \quad & x = F(m_{j_0})\alpha, y = F(m_{j_1})\alpha, M(m_{j_0})_A f = M(m_{j_1})_A g\end{aligned}$$

then we have

$$(F \otimes_{\mathcal{C}} M)_A \cong (F(1) \times M(1)_A)/\sim'_2,$$

where $\sim'_2$ is an equivalence relation generated by R'_2. By the same way, we can obtain

$$(F \otimes_{\mathcal{C}} M)_O \cong (F(1) \times M(1)_O)/\sim'_1,$$

where $\sim'_1$ is an equivalence relation generated by a relation R'_1 on $F(1) \times M(1)_O$ defined by

$$\begin{aligned}(x, n)R'_1(y, l) \quad \Leftrightarrow \quad & \exists \alpha \in F(2)\ \exists j_0, j_1 \in \{0, 1\} \\ \text{s.t.} \quad & x = F(m_{j_0})\alpha, y = F(m_{j_1})\alpha, M(m_{j_0})_O n = M(m_{j_1})_O l.\end{aligned}$$

Finally,

$$\partial_i^{F \otimes_{\mathcal{C}} M} := (F \otimes_{\mathcal{C}} M)(m_i) : (F \otimes_{\mathcal{C}} M)_A \to (F \otimes_{\mathcal{C}} M)_O$$

for $i = 0, 1$ are defined by $\partial_i^{F \otimes_{\mathcal{C}} M}(x \otimes f) = x \otimes \partial_i^{M(1)} f$.

4.3.1 Tensor Product between Two Intrinsic Motifs

Given two intrinsic motifs $M, N : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$, consider a composition

$$\begin{aligned} R_M \circ R_N(G) &= R_M(\mathrm{Hom}(N(-), G)) \\ &= \mathrm{Hom}(M(-), \mathrm{Hom}(N(-), G)) \end{aligned}$$

for a directed graph G. One might expect that a natural isomorphism

$$\mathrm{Hom}((M \otimes N)(-), G) \cong \mathrm{Hom}(M(-), \mathrm{Hom}(N(-), G))$$

holds. In this section we show that this natural isomorphism can be proved if we define the tensor product $M \otimes N$ appropriately.

In the previous subsection we consider the tensor products between presheaves F on $\mathcal{C}$ and intrinsic motifs $M : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$ on one hand, the tensor product $M \otimes N$ to be defined here is that between two intrinsic motifs on the other hand. However, we make use of the construction in the previous subsection in order to define a tensor product between two intrinsic motifs. The idea is simple. Since directed graphs $M(i)(i = 1, 2)$ can be regarded as presheaves on $\mathcal{C}$, we consider the tensor product between $M(i)$ and N.

Definition 4.5 *Let M, N be intrinsic motifs. We define the tensor product between M and N, denoted by $M \otimes N$, which is a functor $\mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$, as follows. For $i = 1, 2$, we regard $M(i)$ as a presheaf on $\mathcal{C}$ and consider the tensor product $M(i) \otimes_{\mathcal{C}} N$. That is, we define*

$$(M \otimes N)(i) = M(i) \otimes_{\mathcal{C}} N$$

for objects $i = 1, 2$ in $\mathcal{C}$. For morphisms $m_j : 1 \to 2$ $(j = 0, 1)$, we define

$$(M \otimes N)(m_j)_A(x \otimes f) = (M(m_j)_O x) \otimes f,$$
$$(M \otimes N)(m_j)_O(x \otimes n) = (M(m_j)_O x) \otimes n$$

for $x \in M(1)_O$, $f \in N(1)_A$ and $n \in N(1)_O$.

More concretely, $(M \otimes N)(i)$ is a directed graph

$$(M(i)_O \times N(1)_A)/\sim_{i,A} \underset{\partial_0^{(M\otimes N)(i)}}{\overset{\partial_1^{(M\otimes N)(i)}}{\rightrightarrows}} (M(i)_O \times N(1)_O)/\sim_{i,O}$$

for $i = 1, 2$. $\sim_{i,A}$ is generated by a relation $R_{i,A}$ on $M(i)_O \times N(1)_A$ defined by

$$\begin{aligned} (x, f)R_{i,A}(y, g) \quad &\Leftrightarrow \quad \exists \alpha \in M(i)_A \ \exists j_0, j_1 \in \{0, 1\} \\ &\text{s.t.} \quad x = \partial_{j_0}^{M(i)}\alpha, y = \partial_{j_1}^{M(i)}\alpha, N(m_{j_0})_A f = N(m_{j_1})_A g. \end{aligned}$$

$\sim_{i,O}$ is generated by a relation $R_{i,O}$ on $M(i)_O \times N(1)_O$ defined by

$$\begin{aligned} (x, n)R_{i,A}(y, l) \quad &\Leftrightarrow \quad \exists \alpha \in M(i)_A \ \exists j_0, j_1 \in \{0, 1\} \\ &\text{s.t.} \quad x = \partial_{j_0}^{M(i)}\alpha, y = \partial_{j_1}^{M(i)}\alpha, N(m_{j_0})_O n = N(m_{j_1})_O l. \end{aligned}$$

$\partial_j^{(M\otimes N)(i)}$ for $j=0,1$ are defined by

$$\partial_j^{(M\otimes N)(i)} x\otimes f := \partial_j^{M(i)\otimes_C N} x\otimes f = x\otimes \partial_j^{N(1)} f.$$

Let us check that $(M\otimes N)(m_j)$ for $j=0,1$ are homomorphisms of directed graphs. First we prove both maps $(M\otimes N)(m_j)_A$ and $(M\otimes N)(m_j)_O$ are indeed well-defined. We only prove the well-definedness of $(M\otimes N)(m_j)_A$. The well-definedness of $(M\otimes N)(m_j)_O$ can be proved by the same manner. It suffices to show that If $(x,f)R_{1,A}(y,g)$ then

$$(M(m_j)_O x, f)R_{2,A}(M(m_j)_O x, g)$$

holds. Suppose $(x,f)R_{1,A}(y,g)$. Then there exist $\alpha\in M(i)_A$ and $j_0,j_1\in\{0,1\}$ such that

$$x=\partial_{j_0}^{M(i)}\alpha,\ y=\partial_{j_1}^{M(i)}\alpha \text{ and } N(m_{j_0})_A f = N(m_{j_1})_A g.$$

For $\beta = M(m_j)_A\alpha$, we have

$$M(m_j)_O x = M(m_j)_O \partial_{j_0}^{M(1)}\alpha = \partial_{j_0}^{M(2)} M(m_j)_A \alpha = \partial_{j_0}^{M(2)}\beta$$

since $M(m_j)$ is a homomorphism of directed graphs. By the same way, we obtain

$$M(m_j)_O y = \partial_{j_1}^{M(2)}\beta.$$

Therefore the desired relation $(M(m_j)_O x, f)R_{2,A}(M(m_j)_O x, g)$ holds.

Second we prove that the following diagram commutes for $k=0,1$.

$$\begin{array}{ccc} (M\otimes N)(1)_A & \xrightarrow{(M\otimes N)(m_j)_A} & (M\otimes N)(2)_A \\ {\scriptstyle \partial_k^{(M\otimes N)(1)}}\big\downarrow & & \big\downarrow{\scriptstyle \partial_k^{(M\otimes N)(2)}} \\ (M\otimes N)(1)_O & \xrightarrow{(M\otimes N)(m_j)_O} & (M\otimes N)(2)_O \end{array}$$

However, we have

$$\begin{aligned} (M\otimes N)(m_j)_O(\partial_k^{(M\otimes N)(1)} x\otimes f) &= (M\otimes N)(m_j)_O(x\otimes \partial_k^{N(1)} f) \\ &= (M(m_j)_O x)\otimes \partial_k^{N(1)} f \\ &= \partial_k^{(M\otimes N)(2)}((M(m_j)_O x)\otimes f) \\ &= \partial_k^{(M\otimes N)(2)}((M\otimes N)(m_j)_A(x\otimes f)) \end{aligned}$$

for $x\in M(1)_O$ and $f\in N(1)_A$.

It is easy to see that $M\otimes N$ is also an intrinsic motif if M and N are intrinsic motifs. Indeed, for any $x\otimes f\in (M\otimes N)(2)_A$, we can write $x = M(m_j)_O y$ for some $y\in M(1)_O$ since we have

$$M(2)_O \subseteq M(m_0)_O(M(1)_O)\cup M(m_1)_O(M(1)_O).$$

Hence

$$x \otimes f = (M(m_j)_O y) \otimes f = (M \otimes N)(m_j)_A (y \otimes f).$$

This means that

$$(M \otimes N)(2)_A \subseteq (M \otimes N)(m_0)_A((M \otimes N)(1)_A) \cup (M \otimes N)(m_1)_A((M \otimes N)(1)_A).$$

The case for O is similar.

Theorem 4.6 *For intrinsic motifs M, N and a directed graph G, a natural isomorphism between presheaves on $\mathcal{C}$*

$$\mathrm{Hom}((M \otimes N)(-), G) \cong \mathrm{Hom}(M(-), \mathrm{Hom}(N(-), G))$$

holds. In other words,

$$R_{M \otimes N} \cong R_M R_N.$$

Proof. Firs we construct a natural transformation

$$\varphi : \mathrm{Hom}(M(-), \mathrm{Hom}(N(-), G)) \to \mathrm{Hom}((M \otimes N)(-), G).$$

Define components of φ

$$\varphi_i : \mathrm{Hom}(M(i), \mathrm{Hom}(N(-), G)) \to \mathrm{Hom}((M \otimes N)(i), G)$$

for $i = 1, 2$ as follows. For any homomorphism of directed graphs $d : M(i) \to \mathrm{Hom}(N(-), G)$, define new homomorphisms of directed graphs $\varphi_i(d) : (M \otimes N)(i) \to G$ by

$$\varphi_i(d)_A : (M \otimes N)(i)_A \to G_A : x \otimes f \mapsto d_O(x)_A f$$

and

$$\varphi_i(d)_O : (M \otimes N)(i)_O \to G_O : x \otimes n \mapsto d_O(x)_O n.$$

$\varphi_i(d)_A$ is well-defined since if $(x, f) R_{i,A} (y, g)$ then there exist $\alpha \in M(i)_A$ and $j_0, j_1 \in \{0, 1\}$ such that

$$x = \partial_{j_0}^{M(i)} \alpha, \ x = \partial_{j_1}^{M(i)} \alpha \text{ and } N(m_{j_0})_A f = N(m_{j_1})_A g,$$

so we have

$$\begin{aligned}
d_O(x)_A f &= d_O(\partial_{j_0}^{M(i)} \alpha)_A f \\
&= (\partial_{j_0}^{\mathrm{Hom}(N(-),G)} d_A \alpha)_A f \\
&= (d_A(\alpha) \circ N(m_{j_0}))_A f \\
&= d_A(\alpha)_A (N(m_{j_0})_A f) \\
&= d_A(\alpha)_A (N(m_{j_1})_A g) \\
&= (d_A(\alpha) \circ N(m_{j_1}))_A g \\
&= (\partial_{j_1}^{\mathrm{Hom}(N(-),G)} d_A \alpha)_A g \\
&= d_O(\partial_{j_1}^{M(i)} \alpha)_A g = d_O(y)_A g.
\end{aligned}$$

The second and eighth equalities hold since d is a homomorphism of directed graphs and the third and seventh equalities follows from the definition of $\partial_k^{\mathrm{Hom}(N(-),G)}$, that is,

$$\partial_k^{\mathrm{Hom}(N(-),G)} : \mathrm{Hom}(N(2), G) \to \mathrm{Hom}(N(1), G)$$

for $k = 0, 1$ are the composition of $N(m_k)$ from the right. We can check the well-definedness of $\varphi_i(d)_O$ by the same way. Next we check $\varphi_i(d)$ $(i = 1, 2)$ are indeed homorphisms of directed graphs. We would like to show that the following diagram commutes for $k = 0, 1$.

$$\begin{tikzcd}
(M \otimes N)(1)_A \arrow[r, "\varphi_i(d)_A"] \arrow[d, "\partial_k^{(M\otimes N)(1)}"'] & G_A \arrow[d, "\partial_k^G"] \\
(M \otimes N)(1)_O \arrow[r, "\varphi_i(d)_O"] & G_O
\end{tikzcd}$$

However, since $d_O(x)$ is a homomorphism of directed graphs, we have

$$\begin{aligned}
\partial_k^G \varphi_i(d)_A(x \otimes f) &= \partial_k^G(d_O(x)_A f) \\
&= (\partial_k^G \circ d_O(x)_A) f \\
&= (d_O(x)_O \circ \partial_k^{N(1)}) f \\
&= d_O(x)_O(\partial_k^{N(1)} f) \\
&= \varphi_i(d)_O(x \otimes \partial_k^{N(1)} f) \\
&= \varphi_i(d)_O \partial_k^{(M\otimes N)(i)}(x \otimes f).
\end{aligned}$$

Now we show that φ is a natural transformation, that is, the following diagram commutes for $j = 0, 1$.

$$\begin{tikzcd}
\mathrm{Hom}(M(2), \mathrm{Hom}(N(-), G)) \arrow[r, "\varphi_2"] \arrow[d, "(-)\circ M(m_j)"'] & \mathrm{Hom}((M \otimes N)(2), G) \arrow[d, "(-)\circ(M\otimes N)(m_j)"] \\
\mathrm{Hom}(M(1), \mathrm{Hom}(N(-), G)) \arrow[r, "\varphi_1"] & \mathrm{Hom}((M \otimes N)(1), G)
\end{tikzcd}$$

In other words, we shall prove that $\varphi_2(d) \circ (M \otimes N)(m_j) = \varphi_1(d \circ M(m_j))$ for $d \in \mathrm{Hom}(M(2), \mathrm{Hom}(N(-), G))$. For the arrow part, given $x \otimes f \in (M \otimes N)(1)_A$, we have

$$\begin{aligned}
(\varphi_2(d) \circ (M \otimes N)(m_j))_A(x \otimes f) &= \varphi_2(d)_A((M \otimes N)(m_j)_A(x \otimes f)) \\
&= \varphi_2(d)_A((M(m_j)_O x) \otimes f) \\
&= d_O(M(m_j)_O x)_A f \\
&= (d \circ M(m_j))_O(x)_A f \\
&= \varphi_1(d \circ M(m_j))_A(x \otimes f).
\end{aligned}$$

The object part can be proved by the same way.

Next we define a natural transformation ψ in the reverse direction.

$$\psi : \mathrm{Hom}((M \otimes N)(-), G) \to \mathrm{Hom}(M(-), \mathrm{Hom}(N(-), G))$$

Indeed, ψ is proved to be the inverse of φ in what follows. Given a homomorphism of directed graphs $d : (M \otimes N)(i) \to G$, we define new homomorphisms of directed graphs

$$\psi_i(d) : M(i) \to \mathrm{Hom}(N(-), G)$$

for $i = 1, 2$ as follows. First we define

$$\psi_i(d)_A : M(i)_A \to \mathrm{Hom}(N(2), G).$$

For $\alpha \in M(i)_A$, $\psi_i(d)_A(\alpha) \in \mathrm{Hom}(N(2), G)$ must be a homomorphism of directed graphs. Its arrow part is defined by a map $\psi_i(d)_A(\alpha)_A$ which sends each $\gamma \in N(2)_A$ to $d_A((\partial_j^{M(i)}\alpha) \otimes f) \in G_A$ for $f \in N(1)_A$ and $j \in \{0, 1\}$ such that $\gamma = N(m_j)_A f$. The existence of such f and j are guaranteed by the definition of intrinsic motif N. $\psi_i(d)_A(\alpha)_A$ is indeed a well-defined map since if $\gamma = N(m_{j_0})_A f = N(m_{j_1})_A g$ then we have $(\partial_{j_0}^{M(i)}\alpha, f) R_{i,A} (\partial_{j_1}^{M(i)}\alpha, g)$ by the definition of $R_{i,A}$. The object part is defined by a similar manner, that is, $\psi_i(d)_A(\alpha)_O(p) = d_O((\partial_j^{M(i)}\alpha) \otimes n)$ for $n \in N(1)_O$ and $j \in \{0, 1\}$ such that $p = N(m_j)_O(n)$. This map is also well-defined by the definition of $R_{i,O}$.

Let us check that $\psi_i(d)_A(\alpha)$ is a homomorphism of directed graphs, that is, the diagram

$$\begin{array}{ccc} N(2)_A & \xrightarrow{\psi_i(d)_A(\alpha)_A} & G_A \\ {\scriptstyle \partial_k^{N(2)}}\big\downarrow & & \big\downarrow{\scriptstyle \partial_k^G} \\ N(2)_O & \xrightarrow{\psi_i(d)_A(\alpha)_O} & G_O \end{array}$$

commutes for $k = 0, 1$. However,

$$\begin{aligned} \partial_k^G \psi_i(d)_A(\alpha)_A(\gamma) &= \partial_k^G d_A((\partial_j^{M(i)}\alpha) \otimes f) \\ &= d_O \partial_k^{(M \otimes N)(i)}((\partial_j^{M(i)}\alpha) \otimes f) \\ &= d_O((\partial_j^{M(i)}\alpha) \otimes \partial_k^{N(1)} f) \\ &= \psi_i(d)_A(\alpha)_O(N(m_j)_O(\partial_k^{N(1)} f)) \\ &= \psi_i(d)_A(\alpha)_O(\partial_k^{N(2)}\gamma) = \psi_i(d)_A(\alpha)_O \partial_k^{N(2)}(\gamma). \end{aligned}$$

The fifth equality follows from

$$\partial_k^{N(2)}\gamma = \partial_k^{N(2)}(N(m_j)_A f) = N(m_j)_O(\partial_k^{N(1)} f)$$

since $N(m_j)$ is a homomorphism of directed graphs.

On the other hand,

$$\psi_i(d)_O : M(i)_O \to \mathrm{Hom}(N(1), G)$$

is defined by for each $x \in M(i)_O$

$$\psi_i(d)_O(x) : N(1) \to G,$$

which is a homomorphism of directed graphs with maps

$$\begin{array}{rcl} \psi_i(d)_O(x)_A & : & N(1)_A \to G_A : f \mapsto d_A(x \otimes f), \\ \psi_i(d)_O(x)_O & : & N(1)_O \to G_O : n \mapsto d_O(x \otimes n). \end{array}$$

$\psi_i(d)_O(x)$ is a homomorphism of directed graphs. Indeed, the diagram

$$\begin{array}{ccc} N(1)_A & \xrightarrow{\psi_i(d)_O(x)_A} & G_A \\ \partial_k^{N(1)} \Big\downarrow & & \Big\downarrow \partial_k^G \\ N(1)_O & \xrightarrow{\psi_i(d)_O(x)_O} & G_O \end{array}$$

commutes for $k = 0, 1$ since

$$\begin{array}{rcl} \partial_k^G \psi_i(d)_O(x)_A f & = & \partial_k^G d_A(x \otimes f) \\ & = & d_O \partial_k^{(M \otimes N)(i)}(x \otimes f) \\ & = & d_O(x \otimes \partial_k^{N(1)} f) \\ & = & \psi_i(d)_O(x)_O(\partial_k^{N(1)} f) \\ & = & \psi_i(d)_O(x)_O \partial_k^{N(1)} f \end{array}$$

for $f \in N(1)_A$.

Now we prove that $\psi_i(d)$ is a homomorphism of directed graphs. We check that the diagram

$$\begin{array}{ccc} M(i)_A & \xrightarrow{\psi_i(d)_A} & \mathrm{Hom}(N(2), G) \\ \partial_k^{M(i)} \Big\downarrow & & \Big\downarrow (-) \circ N(m_k) \\ M(i)_O & \xrightarrow{\psi_i(d)_O} & \mathrm{Hom}(N(1), G) \end{array}$$

commutes for $k = 0, 1$. We shall show that

$$\psi_i(d)_A(\alpha) \circ N(m_k) = \psi_i(d)_O(\partial_k^{M(i)} \alpha)$$

for $\alpha \in M(i)_A$. For $f \in N(1)_A$, we have

$$\begin{array}{rcl} (\psi_i(d)_A(\alpha) \circ N(m_k))_A f & = & \psi_i(d)_A(\alpha)_A(N(m_k)_A f) \\ & = & d_A((\partial_k^{M(i)} \alpha) \otimes f) \\ & = & \psi_i(d)_O(\partial_k^{M(i)} \alpha)_A f. \end{array}$$

For $n \in N(1)_O$, we also have

$$\begin{aligned}
(\psi_i(d)_A(\alpha) \circ N(m_k))_O n &= \psi_i(d)_A(\alpha)_O(N(m_k)_O n) \\
&= d_O((\partial_k^{M(i)}\alpha) \otimes n) \\
&= \psi_i(d)_O(\partial_k^{M(i)}\alpha)_O n.
\end{aligned}$$

Next our task is to check ψ is indeed a natural transformation. We show that the following diagram commutes for $k = 1, 2$.

$$\begin{array}{ccc}
\mathrm{Hom}((M \otimes N)(2), G) & \xrightarrow{\psi_2} & \mathrm{Hom}(M(2), \mathrm{Hom}(N(-), G)) \\
{\scriptstyle (-)\circ(M\otimes N)(m_k)}\Big\downarrow & & \Big\downarrow{\scriptstyle (-)\circ M(m_k)} \\
\mathrm{Hom}((M \otimes N)(1), G) & \xrightarrow{\psi_1} & \mathrm{Hom}(M(1), \mathrm{Hom}(N(-), G))
\end{array}$$

In other words, we prove that

$$\psi_2(d) \circ M(m_k) = \psi_1(d \circ (M \otimes N)(m_k))$$

for $d \in \mathrm{Hom}((M \otimes N)(2), G)$. First for $\alpha \in M(1)_A$ and $\gamma = N(m_j)_A f \in N(2)_A$,

$$\begin{aligned}
(\psi_2(d) \circ M(m_k))_A(\alpha)_A(\gamma) &= \psi_2(d)_A(M(m_k)_A\alpha)_A(N(m_j)_A f) \\
&= d_A((\partial_j^{M(2)} M(m_k)_A\alpha) \otimes f) \\
&= d_A((M(m_k)_O\partial_j^{M(1)}\alpha) \otimes f) \\
&= d_A((M \otimes N)(m_k)_A((\partial_j^{M(1)}\alpha) \otimes f)) \\
&= (d \circ (M \otimes N)(m_k))_A((\partial_j^{M(1)}\alpha) \otimes f) \\
&= \psi_1(d \circ (M \otimes N)(m_k))_A(\alpha)_A(\gamma).
\end{aligned}$$

Second for $\alpha \in M(1)_A$ and $p = N(m_j)_O n \in N(2)_O$, we have

$$\begin{aligned}
(\psi_2(d) \circ M(m_k))_A(\alpha)_O(p) &= \psi_2(d)_A(M(m_k)_A\alpha)_O(N(m_j)_O n) \\
&= d_O((\partial_j^{M(2)} M(m_k)_A\alpha) \otimes n) \\
&= d_O((M(m_k)_O\partial_j^{M(1)}\alpha) \otimes n) \\
&= d_O((M \otimes N)(m_k)_O((\partial_j^{M(1)}\alpha) \otimes n)) \\
&= (d \circ (M \otimes N)(m_k))_O((\partial_j^{M(1)}\alpha) \otimes n) \\
&= \psi_1(d \circ (M \otimes N)(m_k))_A(\alpha)_O(p).
\end{aligned}$$

Third for $x \in M(1)_O$ and $f \in N(1)_A$,

$$\begin{aligned}
(\psi_2(d) \circ M(m_k))_O(x)_A f &= \psi_2(d)_O(M(m_k)_O x)_A f \\
&= d_A((M(m_k)_O x) \otimes f) \\
&= d_A \circ (M \otimes N)(m_k)_A(x \otimes f) \\
&= (d \circ (M \otimes N)(m_k))_A(x \otimes f) \\
&= \psi_1(d \circ (M \otimes N)(m_k))_O(x)_A f.
\end{aligned}$$

Finally, for $x \in M(1)_O$ and $n \in N(1)_O$,

$$\begin{aligned}
(\psi_2(d) \circ M(m_k))_O(x)_O n &= \psi_2(d)_O(M(m_k)_O x)_O n \\
&= d_O((M(m_k)_O x) \otimes n) \\
&= d_O \circ (M \otimes N)(m_k)_O(x \otimes n) \\
&= (d \circ (M \otimes N)(m_k))_O(x \otimes n) \\
&= \psi_1(d \circ (M \otimes N)(m_k))_O(x)_O n.
\end{aligned}$$

φ and ψ are the inverse of each other. Given a homomorphism of directed graphs $d : (M \otimes N)(i) \to G$, first let us prove $\varphi_i \circ \psi_i(d) = d$ for $i = 1, 2$. For $x \otimes f \in (M \otimes N)(i)_A$, we have

$$\varphi_i \circ \psi_i(d)_A(x \otimes f) = \psi_i(d)_O(x)_A(f) = d_A(x \otimes f).$$

Similarly,

$$\varphi_i \circ \psi_i(d)_O(x \otimes n) = \psi_i(d)_O(x)_O(n) = d_O(x \otimes n)$$

for $x \otimes n \in (M \otimes N)(i)_O$. Second we prove that $\psi_i \circ \varphi_i(d) = d$ for any homomorphism of directed graph $d : M(i) \to \mathrm{Hom}(N(-), G)$. For $\alpha \in M(i)_A$ and $\gamma = N(m_j)_A f \in N(2)_A$, we have

$$\begin{aligned}
\psi_i \circ \varphi_i(d)_A(\alpha)_A(\gamma) &= \varphi_i(d)_A((\partial_j^{M(i)}\alpha) \otimes f) \\
&= d_O(\partial_j^{M(i)}\alpha)_A f \\
&= (\partial_j^{\mathrm{Hom}(N(-),G)} d_A \alpha)_A f \\
&= (d_A(\alpha) \circ N(m_j))_A f \\
&= d_A(\alpha)_A(N(m_j)_A f) = d_A(\alpha)_A(\gamma).
\end{aligned}$$

For $\alpha \in M(i)_A$ and $p = N(m_j)_O n \in N(2)_O$,

$$\begin{aligned}
\psi_i \circ \varphi_i(d)_A(\alpha)_O(p) &= \varphi_i(d)_O((\partial_j^{M(i)}\alpha) \otimes n) \\
&= d_O(\partial_j^{M(i)}\alpha)_O n \\
&= (\partial_j^{\mathrm{Hom}(N(-),G)} d_A \alpha)_O n \\
&= (d_A(\alpha) \circ N(m_j))_O n \\
&= d_A(\alpha)_O(N(m_j)_O n) = d_A(\alpha)_O(p).
\end{aligned}$$

For $x \in M(i)_O$ and $f \in N(1)_A$,

$$\begin{aligned}
\psi_i \circ \varphi_i(d)_O(x)_A f &= \varphi_i(d)_A(x \otimes f) \\
&= d_O(x)_A f.
\end{aligned}$$

Finally for $x \in M(i)_O$ and $f \in N(1)_A$, we have

$$\begin{aligned}
\psi_i \circ \varphi_i(d)_O(x)_O n &= \varphi_i(d)_O(x \otimes n) \\
&= d_O(x)_O n.
\end{aligned}$$

This completes the proof of the theorem.

□

Since the composition of R_M is associative, theorem 4.6 implies

Corollary 4.7 *The tensor product between intrinsic motifs is associative.*

Note that since $L_N L_M$ is a left adjoint to $R_M R_N \cong R_{M\otimes N}$, we also obtain

$$L_N L_M \cong L_{M\otimes N}.$$

4.3.2 Examples of Calculation

In this section we demonstrate how the tensor product between intrinsic motifs is useful to determine directed graphs G such that $R_M L_M(G) \cong G$ for some intrinsic motif M. First we present two examples of calculation of the tensor product.

Example 1. Let M be an intrinsic motif consisting of the following data:

$$\begin{aligned} M(2) &= x \xrightarrow{\alpha} y \xrightarrow{\beta} z, \\ M(1) &= x' \xrightarrow{\alpha'} y', \end{aligned}$$

and homomorphisms of directed graphs $M(m_j) : M(1) \to M(2)$ $(j = 0, 1)$ that are determined by $M(m_0)_A(\alpha') = \alpha,\ M(m_1)_A(\alpha') = \beta$. We calculate $M \otimes M$. By the definition of tensor product, $(M \otimes M)(2) =$

$$(M(2)_O \times M(1)_A)/\sim_{2,A} \underset{\partial_0^{(M\otimes M)(2)}}{\overset{\partial_1^{(M\otimes M)(2)}}{\rightrightarrows}} (M(2)_O \times M(1)_O)/\sim_{2,O}.$$

For the set of arrows, we have

$$M(2)_O \times M(1)_A = \{(x, \alpha'), (y, \alpha'), (z, \alpha')\}.$$

By the definition of $R_{2,A}$, we obtain

$$M(2)_O \times M(1)_A \cong (M(2)_O \times M(1)_A)/\sim_{2,A}.$$

On the other hand, we have $M(2)_O \times M(1)_O =$

$$\{(x, x'), (y, x'), (z, x'), (x, y'), (y, y'), (z, y')\}.$$

Since

$$M(m_0)_O(y') = M(m_1)_O(x') \text{ and } x = \partial_0^{M(2)}\alpha,\ y = \partial_1^{M(2)}\alpha,$$

$(x, y')R_{2,O}(y, x')$ holds. Similarly, we have $(y, y')R_{2,O}(z, x')$. Thus we obtain $(M(2)_O \times M(1)_O)/\sim_{2,O}=$

$$\{\{(x, x')\}, \{(x, y'), (y, x')\}, \{(y, y'), (z, x')\}, \{(z, y')\}\}.$$

In summary, $(M \otimes N)(2)$ is a directed graph depicted by

$$\{(x,x')\} \stackrel{(x,\alpha')}{\to} \{(x,y'),(y,x')\} \stackrel{(y,\alpha')}{\to} \{(y,y'),(z,x')\} \stackrel{(x,\alpha')}{\to} \{(z,y')\}.$$

By a similar calculation, we obtain $(M \otimes N)(1)$ as a directed graph

$$\{(x',x')\} \stackrel{(x',\alpha')}{\to} \{(x',y'),(y',x')\} \stackrel{(y',\alpha')}{\to} \{(y',y')\}.$$

$(M \otimes N)(m_j)$ $(j = 0, 1)$ are determined by

$$(M \otimes N)(m_0)_A(x',\alpha') = (x,\alpha'),$$
$$(M \otimes N)(m_0)_A(y',\alpha') = (y,\alpha'),$$

and

$$(M \otimes N)(m_1)_A(x',\alpha') = (y,\alpha'),$$
$$(M \otimes N)(m_1)_A(y',\alpha') = (z,\alpha').$$

Example 2. Let M be the same intrinsic motif in example 1. Let M^n be an intrinsic motif defined by the following data for $n \geq 1$:

$$M^n(2) = 0 \stackrel{0_A}{\to} 1 \stackrel{1_A}{\to} 2 \stackrel{2_A}{\to} \cdots \stackrel{n_A}{\to} n+1,$$
$$M^n(1) = 0 \stackrel{0_A}{\to} 1 \stackrel{1_A}{\to} 2 \stackrel{2_A}{\to} \cdots \stackrel{(n-1)_A}{\to} n$$

and homomorphisms of directed graphs $M^n(m_j)$ $(j = 0, 1)$ defined by

$$M^n(m_0)_A(i_A) = i_A \text{ and } M^n(m_1)_A(i_A) = (i+1)_A$$

for $0 \leq i \leq n$. Note that $M = M^1$. In this example, we shall show that

$$M^n \otimes M \cong M^{n+1}.$$

By the definition of tensor product, $(M^n \otimes M)(2) =$

$$(M^n(2)_O \times M(1)_A)/\sim_{2,A} \underset{\partial_0^{(M^n \otimes M)(2)}}{\overset{\partial_1^{(M^n \otimes M)(2)}}{\rightrightarrows}} (M^n(2)_O \times M(1)_O)/\sim_{2,O}.$$

As in example 1, the set of arrows is just the set

$$M^n(2)_O \times M(1)_A = \{(0,0_A),(1,0_A),\cdots,(n+1,0_A)\}.$$

On the other hand, for the set of objects, since we have $M(m_0)_O(1) = M(m_1)_O(0)$ and

$$i = \partial_0^{M^n(2)} i_A, \; i+1 = \partial_1^{M^n(2)} i_A$$

for $i = 0, 1, \cdots, n$, we obtain

$$(i,1)R_{2,O}(i+1,0)$$

for $i = 0, 1, \cdots, n$. Thus the set of objects is

$$\{\{(0,0)\}, \{(1,0),(0,1)\}, \{(2,0),(1,1)\}, \cdots, \{(n+1,0),(n,1)\}, \{(n+1,1)\}\}.$$

In summary, $(M^n \otimes M)(2)$ is a directed graph depicted by

$$\{(0,0)\} \overset{(0,0_A)}{\to} \{(1,0),(0,1)\} \overset{(1,0_A)}{\to} \cdots \overset{(n,0_A)}{\to} \{(n+1,0),(n,1)\} \overset{(n+1,0_A)}{\to} \{(n+1,1)\}.$$

By a similar argument, we obtain $(M^n \otimes M)(1)$ as a directed graph

$$\{(0,0)\} \overset{(0,0_A)}{\to} \{(1,0),(0,1)\} \overset{(1,0_A)}{\to} \cdots \overset{(n,0_A)}{\to} \{(n,0),(n-1,1)\} \overset{(n,0_A)}{\to} \{(n,1)\}.$$

$(M^n \otimes M)(m_j)$ $(j = 0, 1)$ are determined by

$$(M^n \otimes M)(m_0)_A(i, 0_A) = (i, 0_A),$$
$$(M^n \otimes M)(m_1)_A(i, 0_A) = (i+1, 0_A)$$

for $0 \leq i \leq n$.

Now let us define a natural transformation $\mu_n : M^n \to M^{n+1}$ by

$$\mu_n(1)_A(i_A) = i_A$$

for $0 \leq i \leq n-1$ and

$$\mu_n(2)_A(i_A) = i_A$$

for $0 \leq i \leq n$. In order to see μ_n is indeed a natural transformation, it suffices to show that the diagram

$$\begin{array}{ccc} M^n(2) & \xrightarrow{\mu_n(2)} & M^{n+1}(2) \\ {\scriptstyle M^n(m_1)}\uparrow & & \uparrow{\scriptstyle M^{n+1}(m_1)} \\ M^n(1) & \xrightarrow{\mu_n(1)} & M^{n+1}(1) \end{array}$$

commutes. However, we have

$$\mu_n(2)_A(M^n(m_1)_A(i_A)) = (i+1)_A = M^{n+1}(m_1)_A(\mu_n(1)_A(i_A))$$

for $i = 0, 1, \cdots n-1$. Thus we obtain an infinite chain diagram

$$M \overset{\mu_1}{\to} M^2 \overset{\mu_2}{\to} \cdots \overset{\mu_{n-1}}{\to} M^n \overset{\mu_n}{\to} M^{n+1} \overset{\mu_{n+1}}{\to} \cdots.$$

We can prove that a colimit for the above diagram is an intrinsic motif M^∞ consisting of the following data:

$$M^\infty(2) = 0 \stackrel{0_A}{\to} 1 \stackrel{1_A}{\to} 2 \stackrel{2_A}{\to} \cdots ,$$
$$M^\infty(1) = 0 \stackrel{0_A}{\to} 1 \stackrel{1_A}{\to} 2 \stackrel{2_A}{\to} \cdots$$

and $M^\infty(m_j)$ $(j = 0, 1)$ are homomorphisms of directed graphs determined by

$$M^\infty(m_0)_A(i_A) = i_A,\ M^\infty(m_1)_A(i_A) = (i+1)_A$$

for $i = 0, 1, 2, \cdots$. Indeed, if we define natural transformations

$$\nu_n : M^n \to M^\infty\ (n = 1, 2, \cdots)$$

by $\nu_n(k)_A(i_A) = i_A$ $(k = 1, 2)$ for $i = 0, 1, 2, \cdots$ then we have

$$\nu_{n+1} \circ \mu_n = \nu_n.$$

Suppose there exists a functor $N : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$ with natural transformations $\nu'_n : M^n \to M^\infty$ such that $\nu'_{n+1} \circ \mu_n = \nu'_n$. We would like to show that there exists a unique natural transformation

$$\eta : M^\infty \to N$$

such that $\eta \circ \nu_n = \nu'_n$ for $n = 1, 2, \cdots$. However, if such a η exists then

$$\eta(k)_A \circ \nu_n(k)_A(i_A) = \nu'_n(k)_A(i_A)$$

must hold for $i = 0, 1, \cdots, n-1$ (or $i = 0, 1, \cdots, n$) if $k = 1$ (or $k = 2$), respectively. Thus we uniquely define η by $\eta(k)_A(i_A) = \nu'_n(k)_A(i_A)$ for $i = 0, 1, 2, \cdots$ by choosing sufficiently large n for each i_A (if $k = 1$ then n should satisfy $0 \le i \le n-1$ and if $k = 2$ then n should satisfy $0 \le i \le n$). We can check that η is well-defined by using the equation $\nu'_{n+1} \circ \mu_n = \nu'_n$.

In what follows, we determine all finite connected directed graphs F in the category $\mathcal{H}$ such that $R_{M^\infty} L_{M^\infty}(F) \cong F$. We will see that they are cycles. Recall that a directed graph F is in $\mathcal{H}$ if for any $x \in F_O$ there exist $f, g \in F_A$ such that $\partial_1^F f = x = \partial_0^F g$.

Lemma 4.8 *Let F be a finite connected directed graph in $\mathcal{H}$. Then there exists $n \ge 0$ such that $L_{M^n}(F) \cong L_{M^{n+1}}(F)$. In particular, $L_{M^n}(F)$ is a cycle.*

Proof. First note that L_M is isomorphic to the functor L in chapter 2. Thus $L_{M^n} \cong L_M^n \cong L^n$ for $n \ge 1$. If F is a finite connected directed graph in $\mathcal{H}$ then it is easy to see that $L(F)$ is also a finite connected directed graph in $\mathcal{H}$. Since F is in $\mathcal{H}$, $L(F)$ can be considered as a directed graph consisting of the following data:

$$L(F)_A = F_O,\ L(F)_O = F_A/\sim,$$

where $\sim$ is an equivalence relation generated by a relation R on F_A defined by

$$fRg \Leftrightarrow \partial_0^F f = \partial_0^F g \text{ or } \partial_1^F f = \partial_1^F g.$$

The source and target maps are defined by for $x \in F_O = L(F)_A$,

$$\partial_i^{L(F)} x = [f]$$

if $\partial_i^F f = x$, where $[f]$ is the equivalence class which contains f. These maps are well-defined maps by the definitions of $\mathcal{H}$ and R.

For each $x \in F_O$ choose an arrow $f_x \in \partial_0^{F^{-1}} x$. Since this defines an injective map from F_O to F_A, we conclude that $\#F_A \geq \#F_O = \#L(F)_A$. In general we have $\#L^k(F)_A \geq \#L^{k+1}(F)_A$ for $k = 0, 1, 2, \cdots$. Since F_A is a finite set, there exists $n \geq 0$ such that $\#L^n(F)_A = \#L^{n+1}(F)_A$. For such n we again denote $L^n(F)$ by F. Then $\#F_A = \#L(F)_A = \#F_O$. Since

$$F_A = \cup_{x \in F_O} \partial_i^{F^{-1}}(x)$$

for $i = 0, 1$ and the right hand sides are direct sums, $\#\partial_i^{F^{-1}}(x) = 1$ for any $x \in F_O$ and $i = 0, 1$. Indeed, since F is in $\mathcal{H}$, $\partial_i^{F^{-1}}(x) \geq 1$ for any $x \in F_O$. Hence if there exists $x \in F_O$ such that $\partial_i^{F^{-1}}(x) \geq 2$ then there must exist $x \neq y \in F_O$ such that $\partial_i^{F^{-1}}(y) = 0$. But this is impossible. Thus F must be a direct sum of cycles, however, since F is connected, it is indeed a cycle. Finally note that $L(F) \cong F$ for any cycle F.

□

Let F be a finite connected directed graph in $\mathcal{H}$. By theorem 4.1, $L_{(-)}$ preserves colimits. Hence L_{M^∞} is a colimit for the diagram

$$L_M \overset{L_{\mu_1}}{\to} L_{M^2} \overset{L_{\mu_2}}{\to} \cdots \overset{L_{\mu_{n-1}}}{\to} L_{M^n} \overset{L_{\mu_n}}{\to} L_{M^{n+1}} \overset{L_{\mu_{n+1}}}{\to} \cdots .$$

However, by lemma 4.8, there exists $n \geq 0$ such that $L_{M^n}(F) \cong L_{M^{n+1}}(F)$ and $L_{M^n}(F)$ is a cycle. Therefore we obtain $L_{M^n}(F) \cong L_{M^\infty}(F)$ for such n. Since it is easy to see that $R_{M^\infty}(G) \cong G$ for any cycle G, $R_{M^\infty} L_{M^\infty}(F)$ is a cycle. On the other hand, we can also show that $L_{M^\infty}(G) \cong G$ for any cycle G. Thus a finite connected directed graph F in $\mathcal{H}$ is a cycle if and only if $R_{M^\infty} L_{M^\infty}(F) \cong F$.

4.4 Concluding Remarks

Here we provide some mathematical comments.

Definition 4.5 works for any functors $M, N : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$. Then the unit of the tensor product is $I : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$ with

$$I(2) = \{0 \to 1\},\ I(1) = \{\bullet\}$$

and $I(m_j)_O(\bullet) = j$ $(j = 0, 1)$.

Theorem 4.6 will be extended to an adjunction on the functor category $\mathcal{F}unc(\mathcal{C}, \mathcal{S}ets^{\mathcal{C}^{op}})$. Indeed, we can define a Hom between two functors $N, L : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$ by

$$\mathrm{Hom}(N, L)(i) = \mathrm{Hom}(N(-), L(i)) \quad (i = 1, 2).$$

Then we will obtain a generalization of Cartesian closedness

$$\mathrm{Hom}(M \otimes N, L) \cong \mathrm{Hom}(M, \mathrm{Hom}(N, L))$$

for functors $M, N, L : \mathcal{C} \to \mathcal{S}ets^{\mathcal{C}^{op}}$.

Tensor products in $\mathcal{F}unc(\mathcal{C}, \mathcal{S}ets^{\mathcal{C}^{op}})$ are non-commutative in general. Readers can verify that the tensor product between (3) and (5) in section 4.2 is not commutative.

We conclude this section by the following observation. The condition that $\eta_F : F \to R_M L_M(F)$ is an isomorphism is similar to the condition of sheaf on a topological space. Indeed, if we assume that $M(i)_O = \cup_{j=1,2} \partial_j^{M(i)}(M(i)_A)$ for $i = 1, 2$ then the similarity is clear as we explain bellow.

Components of η_F are

$$(\eta_F)(i) : F(i) \to \mathrm{Hom}(M(i), F \otimes_{\mathcal{C}} M) : \alpha \mapsto \alpha \otimes (-),$$

$(i = 1, 2)$, where $\alpha \times (-) : M(i) \to F \otimes_{\mathcal{C}} M$ is a homomorphism of directed graphs defined by

$$\begin{aligned} (\alpha \otimes (-))_A f &= \alpha \otimes f \text{ for } f \in M(i)_A, \\ (\alpha \otimes (-))_O n &= \alpha \otimes n \text{ for } n \in M(i)_O. \end{aligned}$$

Let us consider what the elements of $\mathrm{Hom}(M(i), F \otimes_{\mathcal{C}} M)$ are. A homomorphism of directed graphs $d : M(i) \to F \otimes_{\mathcal{C}} M$ satisfies

$$\partial_j^{F \otimes_{\mathcal{C}} M} d_A = d_O \partial_j^{M(i)}.$$

The map d determines an element $(d_A(f))_f \in \prod_{f \in M(i)_A} (F \otimes_{\mathcal{C}} M)_A$. By the above equation, if $\partial_j^{M(i)} f = \partial_k^{M(i)} g$ then

$$\partial_j^{F \otimes_{\mathcal{C}} M} d_A(f) = d_O \partial_j^{M(i)} f = d_O \partial_k^{M(i)} g = \partial_k^{F \otimes_{\mathcal{C}} M} d_A(g).$$

On the other hand, consider an element $(\sigma_f)_f \in \prod_{f \in M(i)_A} (F \otimes_{\mathcal{C}} M)_A$ such that if $\partial_j^{M(i)} f = \partial_k^{M(i)} g$ then $\partial_j^{F \otimes_{\mathcal{C}} M} \sigma_f = \partial_k^{F \otimes_{\mathcal{C}} M} \sigma_g$. We can define a homomorphism of directed graphs $d : M(i) \to F \otimes_{\mathcal{C}} M$ by

$$d_A(f) = \sigma_f, \quad d_O(\partial_j^{M(i)} f) = \partial_j^{F \otimes_{\mathcal{C}} M} \sigma_f.$$

d_O is well-defined if we assume that $M(i)_O = \cup_{j=1,2} \partial_j^{M(i)}(M(i)_A)$. By the condition on σ_f, we have

$$\partial_j^{F \otimes_{\mathcal{C}} M} d_A(f) = \partial_j^{F \otimes_{\mathcal{C}} M} \sigma_f = d_O(\partial_j^{M(i)} f).$$

Thus d is a homomorphism of directed graphs.

From the above argument, we can rewrite the condition that η_F is an isomorphism as the following condition SL (Sheaf-Like).

SL The following diagram is a diagram of equalizer for $i = 1, 2$.

$$F(i) \xrightarrow{e} \prod_{f \in M(i)_A} (F \otimes_{\mathcal{C}} M)_A \underset{q}{\overset{p}{\rightrightarrows}} \prod_{\substack{(f,g,j,k) \in M(i)_A^2 \times \{0,1\}^2, \\ \partial_j^{M(i)} f = \partial_k^{M(i)} g}} (F \otimes_{\mathcal{C}} M)_O,$$

where $e(\alpha) = (\alpha \otimes f)_f$, $p((\sigma_f)_f) = (\partial_j^{F \otimes_{\mathcal{C}} M} \sigma_f)_{(f,g,j,k)}$ and $p((\sigma_f)_f) = (\partial_k^{F \otimes_{\mathcal{C}} M} \sigma_g)_{(f,g,j,k)}$.

The similarity with the condition of sheaf on a topological space is immediate. Let $(X, \mathcal{O})$ be a topological space. $\mathcal{O}$ is a partially ordered set consisting of open sets in X by set inclusion, which can be seen as a category. Let F be a presheaf on X, that is, a functor from $\mathcal{O}^{op}$ to $\mathcal{S}ets$. F is called sheaf on X if for any open set $U \subseteq X$ and any open cover $\{U_i\}_{i \in I}$ of U the following diagram is a diagram of equalizer,

$$F(U) \xrightarrow{e} \prod_{i \in I} F(U_i) \underset{q}{\overset{p}{\rightrightarrows}} \prod_{(i,j) \in I^2} F(U_i \cap U_j),$$

where $e(f) = (f|_{U_i})_i$, $p((f_i)_i) = (f_i|_{U_i \cap U_j})_{(i,j)}$ and $p((f_i)_i) = (f_j|_{U_i \cap U_j})_{(i,j)}$.

The similarity is not superficial. Indeed, we can construct bundles on M. The notion of étale-like corresponding to étale map in ordinary sheaf theory can be defined. We can prove an equivalence of category between the category of sheaf-like directed graphs with respect to M and the category of étale-like bundles on M. This issue will be presented elsewhere.

Chapter 5

An Algebraic Description of Development of Hierarchy

We propose an algebraic description of emergence of new levels in trophic level networks. Trophic level networks are described by directed graphs. Their properties are surveyed in terms of an adjunction on a subcategory of the category of directed graphs. In particular, it is shown that trophic level networks are invariant under the composition of the right adjoint functor and the left adjoint functor. This invariance of trophic level networks can be broken by introducing the notion of time into the left adjoint functor. This leads to changes in trophic level networks. We show that the left adjoint functor consists of an intra-level process and an inter-level process. An inconsistency between them arises by the introduction of time. Negotiation between the intra-level process and the inter-level process can resolve the inconsistency at a level, however, a new inconsistency can arises at an emerged new level. Thus our algebraic description can follow indefinite development of trophic hierarchy.

5.1 Introduction

Ecosystems consist of biotic communities, abiotic factors and interrelationships between them. Interrelationships in an ecosystem are often characterized by energy flows between taxa [106, 108]. In particular, hierarchical nature of an ecosystem can be revealed by focusing on a trophic level network [106]. As an ecosystem develops, new trophic levels emerges from the existing trophic level network. Statistical physicists often define emergence of new trophic levels by a stochastic process [14]. However, the purpose of this chapter is providing an algebraic description of such emergence of hierarchy.

Trophic level networks can be described by directed graphs as other many biological or social networks can be [34, 36, 115]. The directed graph representation primarily emphasizes the timeless structure of a network, on which certain dynamics of energy flows occurs. It is convenient to introduce a framework in which common properties of directed graphs structure can be investigated. Category theory [52] provides such a framework. In section 2 we work with the category of directed graphs in order to survey algebraic properties of trophic level networks. However, changes in trophic level networks cannot be treated by focusing on only its timeless structure. The implicit assumption of the categorical treatment of directed graphs is globally controlled synchronization of interrelationships between energy flows. This is unrealistic since all physically realizable interactions take finite time [56]. Interrelationships between energy flows undergo not a global control but local regulations [57]. The notion of time is needed in order to address local regulations of energy flows.

The introduction of time into directed graph framework leads to a distinction between an intra-level process and an inter-level process. Since any consistency between the two processes are not guaranteed a priori, an inconsistency can arise. Negotiation between the intra-level process and the inter-level process toward a consistency attempts to remove inconsistency. However, negotiation itself can generate a new inconsistency by its local character [24, 27, 56]. Thus trophic level networks can undergo changes indefinitely. Since any concrete change in a system occurs under some constraints, what constraints are available in trophic level networks should be addressed [71, 93]. We will show that under an appropriate realistic constraint we can follow a development of trophic hierarchy by our algebraic setting.

This chapter is organized as follows. In section 2 we review a categorical treatment of directed graphs in terms of an adjunction [29]. Trophic level networks are defined as directed graphs and their responses to the adjunction are concerned. In section 3 the notion of time is introduced in order to address changes in trophic level networks. In section 4 we discuss how emergence of new trophic levels can be described by our algebraic formalism. Finally we give conclusions in section 5.

5.2 Duality between Decomposition and Gluing

Organizations of biological or social systems are often described by graphs. Components (e.g. proteins, genes, metabolites, individuals, populations and so on) in a system are usually represented by nodes and interactions between components are represented by arrows (for example, [34, 36, 115]). Meanwhile there are in general multiple biological components for a single interaction, biological or social networks are indeed hypergraphs in which an arrow can connect more than two nodes. Therefore it is a matter how to derive appropriate graphs from real hypergraphs [4]. However, we here limit ourselves to discussing usual directed graphs since our primary concern in this chapter is trophic level networks that can be described by directed graphs.

A trophic level network can be described by a directed graph. Each node represents a trophic level. A trophic level is defined as distance from producers (i.e. plants) in a ecosystem [106]. The least level consists of plants. Harbivores belong to the second level. They are the primary consumers. Carnivores that

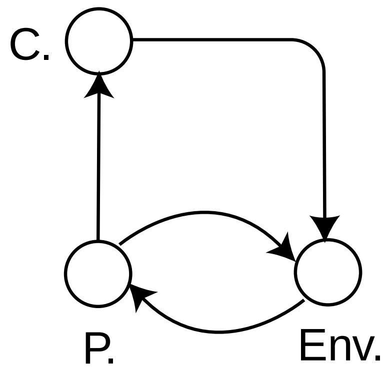

Figure 5.1: A trophic level network consisting of two levels, producers (P.) and the primary consumers (C.). Each level has an energy flow to environment (Env.).

eat harbivores belong to the third level (the secondary consumers). Note that this definition is a functional definition. An individual organism can belong to multiple trophic levels. For example, omnivores belong to more than one trophic level. We put arrows between contiguous levels. The direction of an arrow is from lower to upper level which indicates energy flow. We add another node to the trophic level network that represents environment. Environment includes not only external factors for the ecosystem such as sun light, air, water, soil and other ecosystems but also the detritus food chain in the ecosystem. Hence decomposers belong to environment. Every level has an arrow to environment. There exists an arrow from environment to producers that indicates assimilation of energy from environment. Figure 5.1 shows a trophic level network consisting of producers, the primary consumers and environment.

Directed graphs are formally defined as follows. A quadruplet $G = (A, O, \partial_0, \partial_1)$ is called directed graph. A is a set of arrows. O is a set of nodes. $\partial_i (i = 0, 1)$ are maps from A to O. ∂_0 sends each arrow to its source. ∂_1 sends each arrow to its target. The category of directed graphs $\mathcal{G}rph$ is defined as a category with its objects are directed graphs. The morphisms in $Grph$ are homomorphisms of directed graphs. A homomorphism D between directed graphs $G = (A, O, \partial_0, \partial_1)$ and $G' = (A', O', \partial'_0, \partial'_1)$ is a pair of maps D_A and D_O. D_A is a map from A to A' and D_O is a map from O to O'. They must satisfy the equations $D_O \partial_i = \partial'_i D_A (i = 0, 1)$. That is, homomorphisms of directed graphs are mappings that preserve both sources and targets.

Each node in a directed graph has functions that connect one arrow to another arrow. For example, producers assimilate energy from environment. A part of them are transferred to the primary consumers by their feeding and the remaining parts go back to environment. These two flows are connected to the flow from environment to producers at producers. In order to analyze these functions it is convenient to consider an operation that decompose a node into its functions of connecting arrows [75, 83, 84]. This operation can be defined as a functor from the category of directed graphs $\mathcal{G}rph$ to itself.

The operation of decomposition R is defined as an operation that transforms given directed graph $G = (A, O, \partial_0, \partial_1)$ into a new directed graph $RG = (RA, RO, \partial_0^R, \partial_1^R)$, where

$$\begin{aligned} RA &= \{(f,g) \in A \times A | \partial_1 f = \partial_0 g\} \\ RO &= A \\ \partial_0^R(f,g) &= f \;\; \partial_1^R(f,g) = g \text{ for } (f,g) \in RA. \end{aligned}$$

R is a functor from $\mathcal{G}rph$ to itself.

Each node of a directed graph can be reconstructed by gluing its functions [75]. This operation of gluing can be also defined by a functor. However, a gluing functor cannot be defined on the category of directed graphs $\mathcal{G}rph$. We must concern the operation of gluing on a subcategory of $\mathcal{G}rph$ on which it becomes a functor. A subcategory $\mathcal{H}$ of $\mathcal{G}rph$ is defined as follows. Each object is a directed graph that satisfies the condition that for all $x \in O$ there exist $f, g \in A$ such that $\partial_1 f = x = \partial_0 g$. That is, there exists an incoming arrow and an outgoing arrow for any node. Morphisms of $\mathcal{H}$ are homomorphisms of directed graphs. The gluing operation L that transforms a directed graph $G = (A, O, \partial_0, \partial_1)$ to a new directed graph $LG = (LA, LO, \partial_0^L, \partial_1^L)$ defined as follows is a functor from $\mathcal{H}$ to itself.

$$\begin{aligned} LA &= O \\ LO &= T/\sim \\ T &= \{(x,y) \in O \times O | \exists f \in A \; \partial_0 f = x, \partial_1 f = y\} \end{aligned}$$

$\sim$ is an equivalence relation generated by a relation R on T defined by

$$(x,y)R(z,w) \Leftrightarrow x = z \text{ or } y = w.$$

$\sim$ is the transitive closure of R. That is, $(x,y) \sim (z,w)$ holds if and only if there exist $t_1, t_2, \cdots, t_n \in T$ such that $(x,y) = t_1 R t_2 R \cdots R t_n = (z,w)$. The relation R implies that two arrows are glued if they have a common source or target when G is a binary graph (a directed graph containing at most one arrow between each ordered pair of nodes). Source and target maps are defined as follows.

$$\partial_0^L x = [(\partial_0 f, \partial_1 f)]_\sim \;\; \partial_1^L x = [(\partial_0 g, \partial_1 g)]_\sim$$

where $\partial_1 f = x, \partial_0 g = x,\; f, g \in A$ and $[\alpha]_\sim$ is an equivalence class that includes α. It is proved that $\mathcal{H}$ is the largest subcategory of $\mathcal{G}rph$ on which L becomes a functor. Note that all directed graphs that represent trophic level networks are in $\mathcal{H}$. The functor L can be extended to a functor on $\mathcal{G}rph$ by an appropriate modification, however, we do not concern this aspect in this chapter since it is enough to work on the category $\mathcal{H}$ to discuss emergence of new levels in trophic level networks.

The functors R and L constitute a special kind of duality, called an adjunction.

Theorem 5.1 *L is a left adjoint to R. That is, we have a natural isomorphism*

$$\mathcal{H}(LG, G') \cong \mathcal{H}(G, RG')$$

for any pair of directed graphs G, G', where $\mathcal{H}(G_1, G_2)$ for directed graphs G_1, G_2 is the set of all morphisms from G_1 to G_2 in $\mathcal{H}$.

The proof is given in [29]. See also [80].

By analyzing the adjunction, one can find that the counit $\eta : LR \to I$ of the adjunction is a natural isomorphism, where I is the identity functor on $\mathcal{H}$, which sends each directed graph to itself [29]. That is, for any directed graph G in $\mathcal{H}$ we have a directed graph isomorphism $LRG \cong G$. This means that a directed graph can be fully reconstructed from information about its functions of nodes that connect arrows. Note that the unit $\epsilon : I \to RL$ is not a natural isomorphism. However, we can find a necessary and sufficient condition for $G \cong RLG$ for a directed graph G. Note also that when L is extended to $\mathcal{G}rph$, the counit is not also a natural isomorphism. See [29] for full explanations of these issues. After all the fact that we need in this chapter is that $LRG \cong G$ holds for any directed graph G in $\mathcal{H}$.

Figure 5.2 shows how the trophic level network in Figure 5.1 is recovered by LR. Here producers, the primary consumers and environment are represented by the nodes labeled z, x and y, respectively. Note that both operations of decomposition R and L operate on the whole network simultaneously. The globally controlled synchronization of all the parts of the network is implicitly assumed. This is because they are defined as a mathematical operation, functor. There is no change in a trophic level network as long as the implicit globally controlled synchronization is not removed. However, real trophic level networks do not work in this manner. Synchronization of parts must be achieved by local regulations since it takes a finite duration for parts to interact with each other [56]. In order to formalize local regulations for synchronization between parts, we here focus on the gluing operation. In particular, we introduce the notion of time into the gluing operation. Then the gluing operation becomes a gluing process. In the next section we examine how time can be introduced into the gluing operation.

5.3 Introduction of Time into Gluing Operation

In the following we assume that we are working with binary graphs when we discuss the gluing operation L. Binary graphs are special directed graphs in which there is at most one arrow between an ordered pair of nodes. Note that RG is always a binary graph for any directed graph G. The gluing operation L

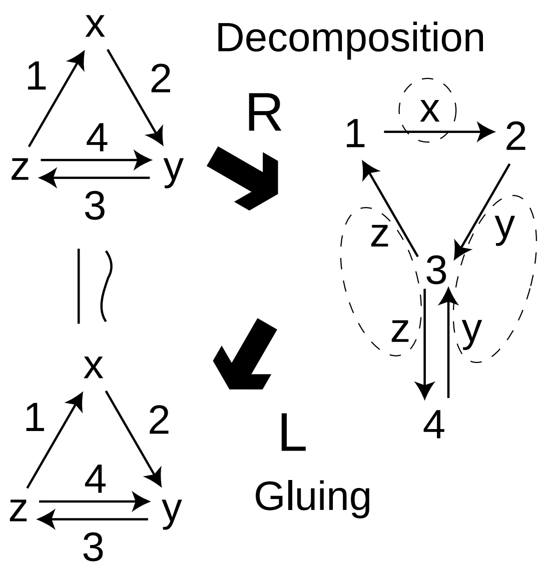

Figure 5.2: The trophic level network in Figure 5.1 is decomposed into functions of connecting arrows (from left to right) by the functor R. The network is reconstructed by gluing the decomposed functions (from right to left), the functor L.

consists of two operations. The first one is gluing arrows by taking the transitive closure of a relation defined on the set of arrows. This operation constructs a set of nodes in a directed graph. A new node is a set of old arrows. The second operation is making new arrows between new nodes. Mathematically this corresponds to defining a source and target maps $\partial_0^L, \partial_1^L$.

Let us suppose these two operations take finite time to complete their works. When we take into account time explicitly we do not say 'operation' but 'process'. Timeless gluing operation L becomes a gluing process. The gluing process is also denoted by L as the gluing operation is. What is the difference between the gluing operation and the gluing process? The gluing operation always reconstructs a given directed graph G in $\mathcal{H}$ from RG, which contains only information about how each node connects arrows in $\mathcal{G}$ due to implicit global synchronization of the whole. On the other hand, the gluing process does not necessarily reconstruct the original directed graph. Suppose that the process of gluing arrows takes d_1 to complete its task and the process of making new arrows between new nodes takes d_2 to complete its task in an arbitrary time unit. If $d_1 \leq d_2$ holds then the process of gluing arrows always finishes before the process of making new arrows between new nodes does. Hence the original directed graph can be reconstructed by the gluing process. On the other hand, if $d_1 > d_2$ then the process of gluing arrows cannot finish before the process of making new arrows between new nodes finishes. Some of old arrows to be glued remain to be unglued. This implies that a node in the original directed graph G are broken up into multiple nodes in LRG, where L is the gluing process. Note that the durations d_1, d_2 just introduced are virtual durations. They are not durations measured in real time. They are defined in order to represent a kind of logical inconsistency in the gluing process.

How can d_1 and d_2 be estimated? Without loss of generality, we can assume that d_2 is a constant since only ratio d_1/d_2 is the matter. Let G be a directed graph in $\mathcal{H}$. The process of gluing arrows in G are defined by the transitive closure of the binary relation R on T. R and T are the same as those defined in section 2. We assume that d_1 correlates with a cost of the process of gluing arrows. If the same computational process is repeated with serial manner and durations between processes can be ignored then time needed to finish all the processes is simply (the number of repeat) $\times$ (time needed to finish a single process). In such a case, the cost of a computational process can be evaluated by the number of computational steps. The transitive closure of a binary relation is an example of this case. Thus we define d_1 by a increasing function of m_G, the maximum of the least number of transition in the transitive closure of R. That is,

$$m_G = \max_{(x,y)\sim(z,w)\in T}\{\min\{n-1|(x,y) = t_1Rt_2R\cdots Rt_n = (z,w)\}\}.$$

For a finite directed graph, it is clear that m_G is always finite. If there exists a directed graph G' in $\mathcal{H}$ such that $G = RG'$ for a directed graph G then the following claim holds.

Theorem 5.2 *$m_{RG} \leq 2$ for any directed graph G in $\mathcal{H}$.*

Proof. Put $G = (A, O, \partial_0, \partial_1)$. By the definitions of R and L,

$$\begin{aligned} RG &= (T, A, \partial_0^R, \partial_1^R), \\ LRG &= (A, T/\sim, \partial_0^{LR}, \partial_1^{LR}), \end{aligned}$$

where $T = \{(f, g) \in A \times A | \partial_1 f = \partial_0 g\}$, $\sim$ is the transitive closure of the binary relation R on T defined by $(f, g)R(k, h) \Leftrightarrow f = k$ or $g = h$. Define two auxiliary relations R_l and R_r on T by

$$(f, g)R_l(k, h) \Leftrightarrow f = k, \quad (f, g)R_r(k, h) \Leftrightarrow g = h.$$

It is clear that $R_l \circ R_l = R_l$ and $R_r \circ R_r = R_r$. Suppose

$$(s_1, t_1)R_l(s_2, t_2)R_r(s_3, t_3)R_l(s_4, t_4)$$

holds. Since we have $s_1 = s_2, t_2 = t_3, s_3 = s_4$ and $(s_i, t_i) \in T$ for $i = 1, 2, 3, 4$,

$$\partial_0 t_1 = \partial_1 s_1 = \partial_1 s_2 = \partial_0 t_2 = \partial_0 t_3 = \partial_1 s_3 = \partial_1 s_4 = \partial_0 t_4.$$

Hence $(s_1, t_4) \in T$ holds. It follows that $R_l \circ R_r \circ R_l \subset R_l \circ R_r$ since we have

$$(s_1, t_1)R_l(s_1, t_4)R_r(s_4, t_4).$$

We can show that $R_r \circ R_l \circ R_r \subset R_r \circ R_l$ by the same way. Thus we obtain $\sim = R_r \cup R_l \cup (R_l \circ R_r) \cup (R_r \circ R_l) = R \cup (R \circ R)$ since $R = R_l \cup R_r$. The claim follows immediately. □

When does the equality $m_{RG} = 2$ hold? Suppose there exists a node that have two incoming arrows and two outgoing arrows in a directed graph G (Figure 5.3 (a), left hand side). In RG, the node is decomposed into four arrows (Figure 5.3 (a), right hand side). Two of them are drawn in parallel and the other two are crossed in Figure 5.3. In order to glue the two parallel arrows we need two transitions of the relation R. Thus if a directed graph G in $\mathcal{H}$ contains such a node it follows that $m_{RG} = 2$. This is ture when either one of the two incoming arrows and either one of the two outgoing arrows are the same (i.e. when a loop is attached to the node with the other incoming and outgoing arrows, Figure 5.3 (b)). On the contrary, if $m_{RG} = 2$ holds then RG must contain one of the two subgraphs shown in Figure 5.3 (c) (left hand side). All three arrows must be distinct although nodes can be degenerated in each case. If the three arrows in each case are glued by the gluing operation L then the corresponding new node has two incoming arrows and two outgoing arrows (Figure 5.3 (c), right hand side). Since $LRG \cong G$ for a directed graph G in $\mathcal{H}$, G must contain a node with two incoming arrows and two outgoing arrows. Since there is no such node in any trophic level network, we have $m_{RG} < 2$ for any directed graph G that represents a trophic level network defined in section 2.

In trophic level networks the process of gluing arrows is an intra-level process and the process of making arrows between nodes is an inter-level process. The inequality $d_1 > d_2$ suggests the existence of an inconsistency between the intra-level process and the inter-level process. In the next section we concern how such an inconsistency arises, can be resolved and leads to development of trophic hierarchy.

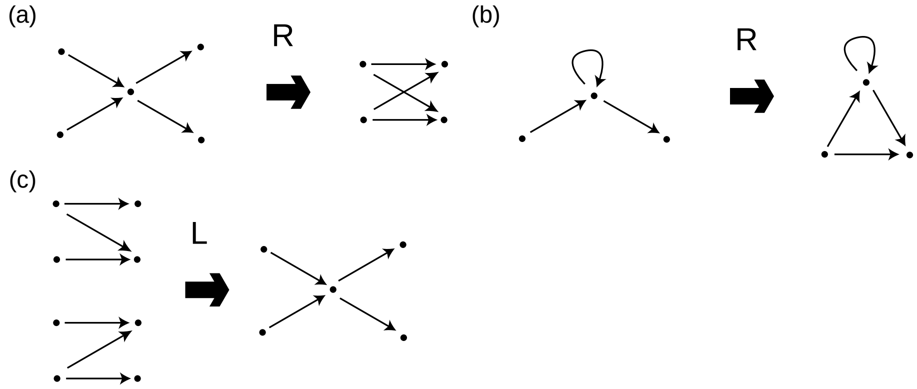

Figure 5.3: (a) If there are two incoming arrows and two outgoing arrows for a node then two transitions of the relation R are necessary in order to glue all arrows that can be glued in RG. (b) Either one of the two incoming arrows and either one of the two outgoing arrows can be the same in (a). (c) L sends both graphs at the left to the same graph.

5.4 Emergence of New Levels

Development of ecosystems can encompass appearances of new trophic levels (Figure 5.4). On the primordial earth there exist trophic level networks consisting of only producers and environment. The producers are prokaryotes. The appearance of eukaryotes indicates the invention of predation, which implies an appearance of a new trophic level, the primary consumers. The secondary consumers come into being along with the organic evolution. In principle, this process of emergence of new levels continues indefinitely. If a geological isolation of a ecosystem is dissolved then a new trophic level can emerge caused by a exogenous factor such as immigration. However, all appearances of new levels cannot be caused by only exogenous factors. For example, the first appearance of the primary consumers in a ecosystem in Precambrian age must have endogenous factors since no exogenous ecological factor is imaginable at this case. Endogenous factors for emergence of new levels are more fundamental than exogenous ones since they work without any exogenous factor.

Without exogenous causes, any new trophic level must be latent in the existing trophic level networks. How can such latency be represented in directed graphs? Since arrows in a trophic level network represents energy flows between nodes (trophic levels and environment), the representation of latency should also be considered in terms of energy flows. It seems that this can be done by adding a loop to a trophic level that represents an intra-level energy flow. On the other hand, by the functional definition of the trophic level, a new trophic level emerges from only the highest level. for example, an appearance of new species of plant does not change the existing trophic level network. Therefore

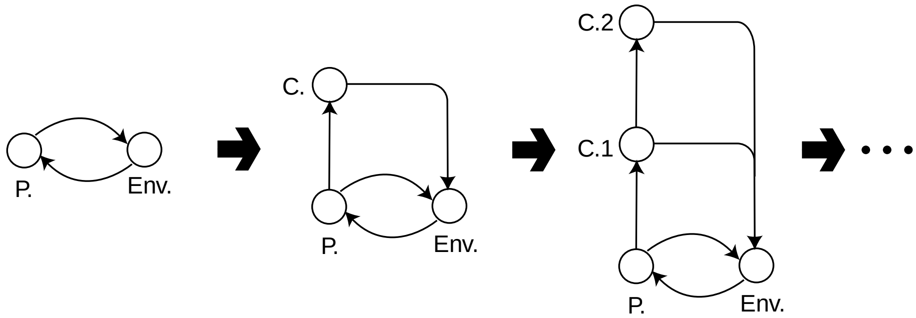

Figure 5.4: Development of trophic hierarchy.

we here suggest that the existence of a latent new level can be represented by adding a loop to the highest level. If a directed graph G in $\mathcal{H}$ that represents a trophic level network is modified in such a way then the value of m_{RG} changes from 0 or 1 to 2. This leads to increase in d_1 the time needed to complete the process of gluing arrows in RG.

The increase in d_1 results in two different situations. The first situation is uninteresting case, the inequality $d_1 \leq d_2$ remains to be held. In this case the gluing process cannot be distinguished from the gluing operation, hence there is no change in the trophic level hierarchy. In the second situation, the inequality $d_1 \leq d_2$ is broken. An inconsistency between the intra-level process of gluing arrows in RG to make nodes in LRG and the inter-level process of making arrows in LRG arises. Since the former is slower than the latter, arrows in RG to be glued remain not to be glued. A node in G must be broken up into multiple nodes in LRG if its function of connecting arrows cannot be fully glued. This is a negotiation between the intra-level process and the inter-level process in order to retain logical consistency. We call such a gluing process the indefinite gluing. There are several possibilities in the shape of the resultant directed graph LRG without any constraint. However, we here imposes a constraint that restrict the possibilities. Since we are interested in development of trophic hierarchy, we assume that the resultant directed graph has a property that all trophic networks have. It is a constraint that any trophic level has a energy flow to environment. In fact we can show that just one possibility is acceptable by this constraint and the resultant directed graph represents a trophic level network in which the number of trophic levels increases by one with a loop at the highest level. We see this by an example in the following.

Let G be a trophic level network that consists of two levels. We assume that without a loop at the highest level $G \cong LRG$ holds where L is the gluing process. In this case we have $m_{RG} = 1$. Hence we also assume that when a loop exists at the highest level (Figure 5.5, left hand side), the gluing of arrows with a single transition of the relation R on the set T of arrows in RG can finish before the process of making arrows between nodes in LRG. Thus two pairs of arrows

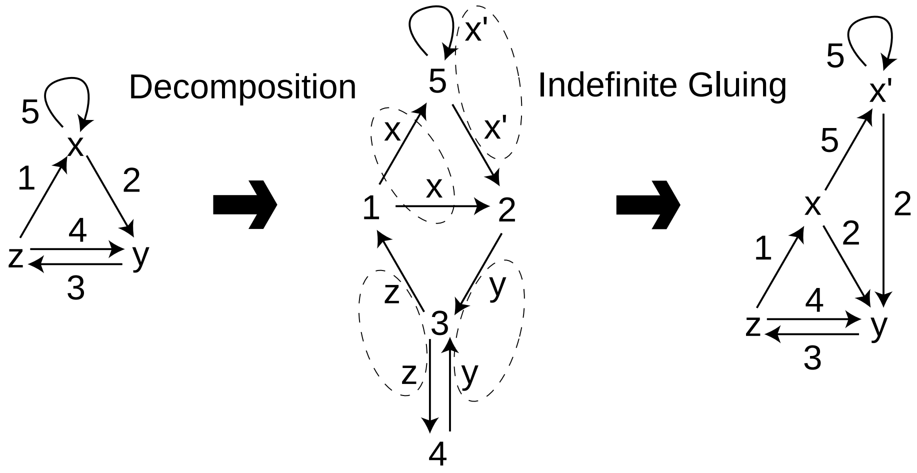

Figure 5.5: The loop at the highest level in the trophic level network at the left hand side indicates a new level is latent in the existing trophic level network. The latent new level emerges explicitly by indefinite gluing.

$\{3 \to 1,\ 3 \to 4\}$ and $\{2 \to 3,\ 4 \to 3\}$ in RG can be glued respectively (Figure 5.5, center). Suppose two arrows $5 \to 2$ and $1 \to 2$ are glued. $1 \to 5$ cannot be glued to them since it needs two transition of R to glue $1 \to 5$ to $5 \to 2$. However, a node in LRG (which is an equivalence class of arrows in RG) containing $1 \to 5$ have no arrows to environment (node 2 represents energy flows to environment). This is impossible because of the assumed constraint. Hence $5 \to 2$ and $1 \to 2$ belong to different equivalence classes. $1 \to 5$ cannot be glued to $5 \to 2$ since the gluing needs two transition of R via $5 \to 5$. If $1 \to 5$ is not glued to $1 \to 2$ then the equivalence class containing $1 \to 5$ does not have any arrow to environment. Hence $1 \to 5$ must be glued to $1 \to 2$. By the similar argument, $5 \to 5$ is glued to $5 \to 2$. Thus we obtain the set of nodes in LRG as $\{x, x', y, z\}$ where $x = \{1 \to 2,\ 1 \to 5\}, x' = \{5 \to 2,\ 5 \to 5\},\ y = \{2 \to 3,\ 4 \to 3\}$ and $z = \{3 \to 1,\ 3 \to 4\}$. Arrows in LRG are defined as follows. Let a, b are nodes in LRG. We put an arrow from a to b if there exists $i \to j$ in a and $k \to l$ in b such that $j = k$. This is consistent with the definition in the gluing operation L. The resultant directed graph is a trophic level network with a loop at the highest level (Figure 5.5, right hand side). The number of levels in LRG increases by one from that in G. Finally note that the process of development of trophic hierarchy described above can continue indefinitely from the simplest network that consists of only producers and environment.

5.5 Conclusions

In this chapter we provided an algebraic description of emergence of trophic hierarchy. Introduction of time into functors gives rise to an inconsistency between an intra-level process and an inter-level process. Negotiation between the intra-level process and the inter-level process under a realistic constraint leads to an appearance of a new level. A new level is latent at the highest level even after the inconsistency between the intra-level process and the inter-level process is resolved at a lower level. Hence development of trophic hierarchy can continue indefinitely in principle.

In real ecosystems, the number of trophic levels is limited by constraints such as the history of community organization, resource availability, the type of predator-prey interactions, disturbance and ecosystem size [79]. Extinctions can decrease the number of trophic levels [81]. Non-trophic effects are important to understand trophic relationships [112]. In our algebraic framework, these issues are included in the question that how the inconsistency between the intra-level process and the inter-level process arises. In this chapter we did not treat this problem and only provided a description that what happens if the inconsistency arises.

Chapter 6

Imbalance and Balancing: Development of Ecological Flow Networks

In this chapter we address balancing process of ecological flow networks. In existing approaches, macroscopic objectives to which systems organize are assumed. Flow balance provides only constraints for the optimization. Since flow balance and objectives are separated from each other, it is impossible to address how the appearance of objectives is related to flow balance. Therefore we take an alternative approach, in which we directly describe a dynamics of balancing process. We propose a simple mathematical formula for local balancing dynamics and show that it can generate a self-organizing property, which could be seen as a primitive objective.

6.1 Introduction

Ecosystems consist of complex networks of energy, materials and services. Various macroscopic indices have been proposed in order to understand complex ecological networks as a whole [95, 114]. They can be roughly classified as follows: indices emphasizing productions in ecosystems [35, 45, 69], indices emphasizing dissipations in ecosystems, [1, 96, 103] and indices emphasizing activities of biological communities and their interrelationships [106, 114]. They are different in details and have advantages respectively, however, they all assume that macroscopic objectives to which systems self-organize. In recent years, similar attempts emerges in understanding biological networks inside an organism such as metabolic or gene transcription regulation networks [9, 31, 39]. As in ecology, they assume macroscopic objectives that are to be maximized or minimized.

The idea that biological systems self-organize toward macroscopic objectives may be useful for systems once established. Indeed, flux balance analysis (FBA) theory makes good predictions on experiments if one can set appropriate objectives [39]. However, appearances of macroscopic objectives cannot be addressed if one assumes them in advance. In order to discuss how macroscopic objectives could emerge we focus on an assumption that the macroscopic objective approach makes. The macroscopic objective approach assumes that a balance between incoming flows to a system and outgoing flows from the system. The flow balance defines constraints under which a macroscopic objective is optimized. The balance and the objective are separated from each other. Here the flow balance is expressed as merely a set of equations that lack the ability of balancing, which can locally regulate flows toward a balance. Macroscopic objectives are introduced in order to compensate for the lack of balancing ability. As an alternative to the macroscopic objective approach, we directly describe the local balancing dynamics by a simple mathematical expression. This alternative approach admits imbalances between incoming and outgoing flows. In this chapter we will discuss a possibility that accumulations of imbalances generate a developmental direction of ecological flow networks.

This chapter is organized as follows. In section 2, we introduce the notion of balancing. In section 3, we present a mathematical formulation of balancing process. In section 4, we give two examples of balancing process. In section 5, we show balancing process can result in a self-organizing property by computer simulation. In section 6, we analyze the mechanism of balancing. Finally, in section 7, we give conclusions.

6.2 From Balance to Balancing

The macroscopic objective approach assumes a balance in flows. For example, the sum of incoming flows to a system must be equal to the sum of outgoing flows from the system for each chemical species. Without this assumption, one may not able to find maximal or minimal points of a macroscopic objective since the domain of the objective function is indefinite. This assumption might be plausible for biological systems that can exist persistently. The intuition that this assumption is plausible might come from the imagination that flow balances are self-regulated as a whole at every moment in persistently existing biological systems. However, if this image is described by mathematics then it becomes merely a set of equations. The image of self-regulation at every moment is killed. Macroscopic objectives are introduced in order to compensate for the lack of the image of self-regulation at every moment. Here the image of self-regulation toward a balance as a whole is separated into two parts, balance equations and an objective function.

Since such a way of description assumes a macroscopic objective in advance, we cannot address a question about how macroscopic objectives could appear. An approach that could get in this question is simply describing the image of self-regulation of flows toward a balance. In this approach we admit the existence of an imbalance between incoming and outgoing flows at each node of a flow network [56]. Flows in a network regulate their size in order to eliminate the imbalances. We call this process *balancing*. However, if balancing works only a local manner then imbalances might be never eliminated. The balancing process would persist indefinitely. We consider the possibility that a local balancing process could induce development of flow networks toward organization. In the next section we introduce a mathematical formulation of this idea.

Imbalance can be seen as a local orientating function of ecosystems, which is not a macroscopic objective but specifies only direction of change of each flow. The idea of orientating function is due to Ulanowicz [108]. At first he propose a quantity called ascendency (which will be reviewed in section 5) as a macroscopic objective of ecosystems [105, 106]. However, he later turned to ascendency as an orientating function of ecosystem, not an objective. This probably arises from internal perspective since ecosystems themselves would never know the global optimums. We enforce the direction of Ulanowicz by focusing on locality [56, 94].

We can compare our approach with the existing approach as follows.

Existing Approach Balance+Objective.

Our Approach Balancing.

The same idea as balancing here is proposed in the study of animal learning behaviors such as sexual imprinting and discrimination learning of mimicry [12, 13, 50, 51]. We briefly explain them as an auxiliary line of understanding. Peak shift is known as the following phenomenon. When animals are trained to discriminate between a positively rewarded stimulus (S+) and a negatively or neutrally rewarded stimulus (S-), we might expect that their responses to novel stimuli are the strongest around the training stimuli. In peak shift, however, animals' responses to novel stimuli are stronger away from the S+ in a direction opposite from the S-, and vice versa.

The research group of ten Cate treats sexual imprinting of male children of a zebra finch [12]. Male children are raised by parents that are sexually dimorphic, different in only beak color. Beaks of fathers in the first experimental group are colored red and that of mothers are colored orange. In the second group, the reverse coloring is done. It is known that when a male raised in this way becomes an adult he prefers females with orange beaks if he belongs to the first group. On the other hand, if he belongs to the second group then he prefers females with red beaks. Thus the beak color of mothers works as S+ and that of fathers works as S-. In the experiment of ten Cate *et al.* [12], the males can choose their mates from eight females whose beaks are colored in different eight stages from more intense red to more yellow orange including two beak colors (i.e. red and orange) of their parents. Males in the first group tend to choose females with more extreme red than their mother on one hand, males in the second group prefer females with more yellow orange than their mother on the other hand. In the other articles, the possibility that peak shifts lead to species discrimination is discussed [13, 51].

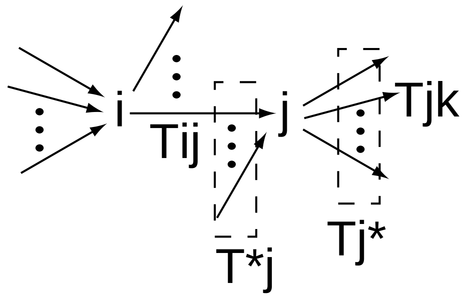

Figure 6.1: Imbalance of flow $i \to j$ at node j.

In general learning is aimed to an acquisition of a specific performance. However, the experiment of ten Cate *et al.* shows that if males try to learn a performance of choosing females with a specific color then the performance itself shifts as a result. This implies that there are biases in males' cognitions. It suggests that an accumulation of the biases in animal cognitions could cause species discrimination.

6.3 Imbalance and Balancing in Flow Networks

Let an ecosystem consist of N nodes (taxa). Let T_{ij} be the size of flow from node i to node j for $1 \leq i, j \leq N$. Total throughput in the system is defined by $T = \sum_{i,j} T_{ij}$. The sum of incoming flows to node i is denoted by $T_{*i} = \sum_k T_{ki}$ and the sum of outgoing flows from node i is denoted by $T_{i*} = \sum_k T_{ik}$. The flow balance at node i is defined by

$$T_{*i} = T_{i*}.$$

As mentioned in section 2, we do not assume flow balance in advance and admit imbalances [57]. Instead of flow balance condition we assume balancing process at each flow. Each flow in a flow network detects an imbalance locally and changes its size in the direction that decreases the imbalance detected.

The definition of imbalance δ_{ij} for flow $i \to j$ is as follows. One of the simplest way is to define imbalance at each node as the difference between the sum of incoming flows and the sum of outgoing flows. In this definition imbalance is defined associated with a node. However, we would like to define imbalance associated with a flow. This is done by considering how an incoming flow to a node is distributed between outgoing flows from the node and how an outgoing flow from a node is contributed by incoming flows to the node. This consideration can be seen as a generalization of an operation called "decomposition into function" in [29].

Let us focus on node j (Figure 6.1). The amount of flow from $i \to j$ to $j \to k$

will be

$$T_{ij} \times \frac{T_{jk}}{T_{j*}}$$

if how obtained materials are utilized is irrelevant to their sources at node j. On the other hand, the contribution of $i \to j$ to T_{jk} will be

$$T_{jk} \times \frac{T_{ij}}{T_{*j}}$$

under the same assumption. Obviously if flow balance is satisfied at node j then these two quantities are equal. So we make use of the absolute value of the difference between them in order to define imbalance associated with a flow. Consider the summation with respect to k :

$$\sum_k T_{ij}T_{jk}|\frac{1}{T_{j*}} - \frac{1}{T_{*j}}| = T_{ij}T_{j*}|\frac{1}{T_{j*}} - \frac{1}{T_{*j}}| = T_{ij}|1 - \frac{T_{j*}}{T_{*j}}|.$$

Moreover we consider imbalance per unit flow by dividing this quantity by T_{ij} :

$$|1 - \frac{T_{j*}}{T_{*j}}|.$$

If we focus on node i then we obtain a quantity

$$|1 - \frac{T_{*i}}{T_{i*}}|$$

by the same way. Let $0 \leq \alpha \leq 1$ be contribution rate of node i. We define an imbalance associated with flow $i \to j$ by

$$\delta_{ij} = \alpha|1 - \frac{T_{*i}}{T_{i*}}| + (1-\alpha)|1 - \frac{T_{j*}}{T_{*j}}|.$$

Balancing process is defined so that each flow changes its size in the direction in which the imbalance associated with it decreases. That is, if the partial differential with respect to T_{ij}

$$\frac{\partial \delta_{ij}}{\partial T_{ij}} = \mathrm{sgn}(T_{i*} - T_{*i})\alpha\frac{T_{*i}}{T_{i*}^2} + \mathrm{sgn}(T_{*j} - T_{j*})(1-\alpha)\frac{T_{j*}}{T_{*j}^2}$$

is negative then the flow increases and if the partial differential is positive then the flow decreases, where $\mathrm{sgn}(x) = +1(x > 0), \mathrm{sgn}(x) = -1(x < 0)$. At present we do not specify precise functional form of flow change but only specify the direction of flow change.

In the next section we analyze two examples by using the above formulation.

6.4 Examples

The first example is from economics. Let us denote the size of material flow from resources to manufacturers by f_0, from manufacturers to merchants by f_1 and from merchants to consumers by f_2.

$$\text{resources} \xrightarrow{f_0} \text{manufacturers} \xrightarrow{f_1} \text{merchants} \xrightarrow{f_2} \text{consumers}$$

We focus on the flow f_1 from manufacturers to merchants. The imbalance associated with this flow and its partial differential with respect to f_1 are

$$\begin{aligned} \delta_1 &= \alpha|1-\frac{f_0}{f_1}| + (1-\alpha)|1-\frac{f_2}{f_1}|, \\ \frac{\partial \delta_1}{\partial f_1} &= \operatorname{sgn}(f_1-f_0)\alpha\frac{f_0}{f_1^2} + \operatorname{sgn}(f_1-f_2)(1-\alpha)\frac{f_2}{f_1^2}. \end{aligned}$$

If $f_1 < f_0, f_2$ then $\operatorname{sgn}(f_1-f_0) = \operatorname{sgn}(f_1-f_2) = -1$. Since $\frac{\partial \delta_1}{\partial f_1} < 0$ for any α, f_1 increases by balancing process independent of α. This can be interpreted as follows. If outgoing flow is greater than incoming flow at merchants then they try to increase incoming flow in order to sell more and at the same time if outgoing flow is less than incoming flow at manufacturers then they try to increase outgoing flow in order to decrease stocks.

If $f_1 > f_0, f_2$ then $\operatorname{sgn}(f_1-f_0) = \operatorname{sgn}(f_1-f_2) = +1$. In this case we have $\frac{\partial \delta_1}{\partial f_1} > 0$. Hence f_1 decreases independent of α. Since production and sales of commodities are restrected by both inflow of resources and amount of consumption, this case is also consistent with our intuition about economics.

Next we consider the case $f_0 < f_1 < f_2$. In this case whether f_1 increases or decreases is dependent on α. The condition in which

$$\frac{\partial \delta_1}{\partial f_1} = \frac{\alpha f_0 - (1-\alpha)f_2}{f_1^2}$$

is negative is

$$f_2 > \frac{\alpha}{1-\alpha} f_0.$$

If $\alpha \leq \frac{1}{2}$ then this condition is always satisfied by the assumption $f_2 > f_0$ and hence f_1 increases. On the other hand, if $\alpha > \frac{1}{2}$ then f_1 increases only if $\frac{f_2}{f_0}$ is greater than $\frac{\alpha}{1-\alpha}$, that is, f_0 is sufficiently smaller than f_2.

If $f_2 < f_1 < f_0$ then the condition in which

$$\frac{\partial \delta_1}{\partial f_1} = \frac{-\alpha f_0 + (1-\alpha)f_2}{f_1^2}$$

is negative is

$$f_2 < \frac{\alpha}{1-\alpha} f_0.$$

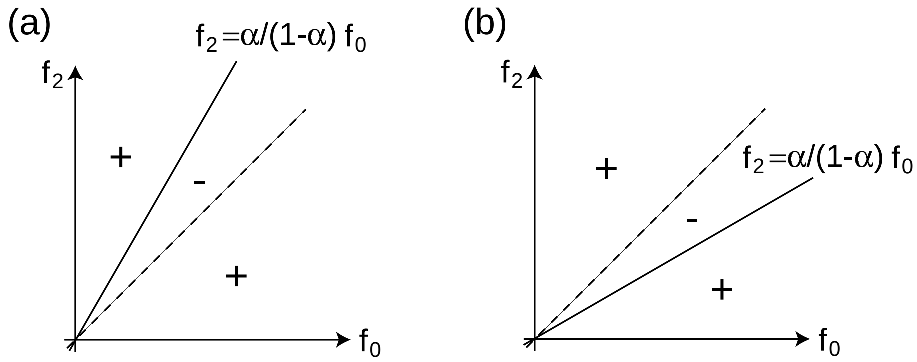

Figure 6.2: $\min\{f_0, f_2\} < f_1 < \max\{f_0, f_2\}$. $+$ indicates the region in which f_1 increases and $-$ indicates the region in which f_1 decreases. (a)$\alpha > \frac{1}{2}$. (b)$\alpha < \frac{1}{2}$.

If $\alpha \geq \frac{1}{2}$ then this is always true and hence f_1 increases. If $\alpha < \frac{1}{2}$ then f_1 increases only if $\frac{f_2}{f_0}$ is smaller than $\frac{\alpha}{1-\alpha}$, that is, f_0 is sufficiently larger than f_2.

Figure 6.2 summarizes the case $\min\{f_0, f_2\} < f_1 < \max\{f_0, f_2\}$. First note that if $0 < \alpha < 1$ and sizes of f_0 and f_2 are chosen independently in the circle centered at the origin then the probability of increase of f_1 is greater than the probability of decrease. In particular, if $f_0 < f_1 < f_2$ then f_1 increases if $\frac{f_2}{f_0}$ is sufficiently large for given α. This means that manufacturers flow more commodities to merchants in order to fulfill the demand of consumers f_2. In this case f_0 must also increase in order manufacturers to survive. If the demand of consumers increases continually then the flow from resources to manufacturers must increase in order to respond to the demand. This would be possible in the knowledge based industries like software business in which one can expect increasing return, not in the resource based industries like heavy industries [5]. For small α, f_1 can increase easily. On the other hand, if α is large then the possibility of increase in f_1 decreases. Thus it seems that small α corresponds to the knowledge based industries that can be pulled by the demand of consumers and large α corresponds to the resource based industries that are largely restricted by resources. Of course we cannot know all aspects of the economic system in terms of balancing process, however, we can see certain aspects through the proposed formulation.

Next example is a simple tritrophic ecosystem consisting of plants, herbivores and carnivores. We denote material flows between them as follows.

$$\text{environment} \xrightarrow{f_0} \text{plants} \xrightarrow{f_1} \text{herbivores} \xrightarrow{f_2} \text{carnivores}$$

In particular here we suppose a tritrophic ecosystem such as consisting of Lima bean, two-spotted spider mites and predatory mites in which plants emit volatiles that attract carnivores when herbivores eat plants [99, 102]. The conditions for increase or decrease in f_1 are the same as in the first example. Carnivores that catch herbivores are bodyguards for plants and carnivores can find their foods by volatiles emitted by plants that attract them. One question arises here. Is there any merit for herbivores in this system? It is known that plants do not emit volatiles that can attract carnivores by physical stimuli only. Plants attract carnivores only if they are subject to chemical stimuli originated from herbivores. Why do herbivores provide chemical stimuli to plants that attract carnivores [99]? On the other hand, Suzuki *et al.* shows that if there is interaction by volatiles then both the number of herbivores and carnivores can increase by computer simulation [102].

Let us answer the question in terms of balancing process. Since plants do not emit volatiles until the amount of chemical stimuli exceeds a certain level, we can assume that $f_0 < f_1$ when they begin to emit volatiles. On the other hand, since if carnivores begin to catch herbivores then the number of herbivores tends to decrease, we assume that $f_1 < f_2$. Hence the situation $f_0 < f_1 < f_2$ appears. In this case if $\frac{f_2}{f_0}$ is greater than a constant dependent on α then f_1 increases by balancing process. This could be a merit for herbivores. How is such a consequence possible in reality? We borrow an explanation by Suzuki *et al.* [102]. As mentioned above, there is a time-lag between start of eating by herbivores and emission of volatiles. Therefore a part of herbivores will be able to move to the other leaves before the arrival of carnivores. Such herbivores will make a new colony on the other leaves. Thus in some cases, the number of herbivores could increase.

From the above two examples, one can see that balancing process could have certain explanatory power. In the next section we present the result of computer simulation based on balancing process on more general flow networks and discuss how the distribution of flows develops.

6.5 Computer Simulation

In this section we discuss balancing process on more general flow networks. We prepare a random network with N nodes We assume that the number of in-degree is the same as the number of out-degree for every node. We denote the number by m. We also assume that there is no self-loop in the random network. Such a setting is not realistic, however, the purpose of this section is to address the properties of balancing process. This setting is adopted in order to facilitate mathematical analysis. In the computer simulation below, $N = 30$ and $m = 10$. So the total number of flows is 300. Furthermore, we assume that $\alpha = \frac{1}{2}$ in this section. The behaviors for different values of α is discussed in the next section. When $\alpha = \frac{1}{2}$ we will show that the flow network has a self-organizing property in the following.

Time evolution of flows is defined by the following stochastic model. Let ϵ

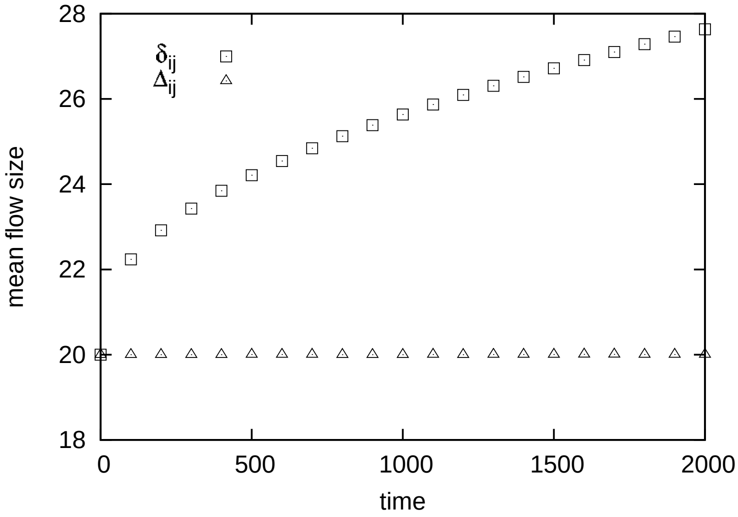

Figure 6.3: Time evolution of mean flow size.

be a uniform random number in $[0, 2\eta]$. We define

$$T_{ij}^{\tau+1} = \begin{cases} T_{ij}^{\tau} + \epsilon & (\frac{\partial \delta_{ij}^{\tau}}{\partial T_{ij}^{\tau}} < 0) \quad (6.1a) \\ T_{ij}^{\tau} - \epsilon & (\frac{\partial \delta_{ij}^{\tau}}{\partial T_{ij}^{\tau}} > 0). \quad (6.1b) \end{cases}$$

The suffix τ indicates quantities at τth period. As a control experiment, we also show results when imbalance is defined by

$$\Delta_{ij} = |T_{*i} - T_{i*}| + |T_{*j} - T_{j*}|.$$

Initial condition is given by a uniform distribution with mean 20 and width 0.1 in both cases. Moreover, $\eta = 0.1$ for both cases. Figure 6.3 shows time evolution of mean flow size. Each point is averaged over 1000 trials. Mean flow size increases when imbalance is given by δ_{ij}. In contrast, it does not increase in the case of Δ_{ij}.

Next we calculate ascendency of the system in order to measure the degree of development of flow networks. Ascendency is first defined as a macroscopic objective of ecosystem organization, afterward re-defined as an orientating function [105, 106, 108]. It is defined for a flow network by the multiplication of total throughput T and mutual information I of the network. Total throughput T is an index of growth of the system on one hand, mutual information I measures how the system is organized. The re-defined version of ascendency hypothesis says that "in the absence of overwhelming external disturbances, living systems exhibit a natural propensity to increase in ascendency" [108]. Note that this statement is derived from empirical observations. From Figure 6.3, we already know that total throughput T increases by balancing process with δ_{ij}. Hence we focus on mutual information I in the following. Mutual information I to be defined here is average information gain between incoming flows and outgoing flows at each node. The a priori probability to find a flow $i \to j$ and its uncertainty are

$$\frac{T_{i*}}{T} \times \frac{T_{*j}}{T}, \ -\log \frac{T_{i*}T_{*j}}{T^2},$$

respectively. On the other hand, the emprical probability to find a flow $i \to j$ and its uncertainty are

$$\frac{T_{ij}}{T}, \ -\log \frac{T_{ij}}{T},$$

respectively. Therefore average information gain (mutual information) I is

$$\sum_{i,j} \frac{T_{ij}}{T}(-\log \frac{T_{i*}T_{*j}}{T^2} - (-\log \frac{T_{ij}}{T})) = \sum_{i,j} \frac{T_{ij}}{T} \log \frac{TT_{ij}}{T_{i*}T_{*j}}.$$

Ascendency is defined by

$$A = T \times I = \sum_{i,j} T_{ij} \log \frac{TT_{ij}}{T_{i*}T_{*j}}.$$

If a distribution of flows is given by $P(t)$ then mutual information I is approximately given by the following formula [107].

$$I = \langle \frac{t}{\langle t \rangle} \log \frac{t}{\langle t \rangle} \rangle + \log \frac{N}{m},$$

where $\langle \cdots \rangle$ is average with respect to P, N is the number of nodes and m is the number of in-degree or out-degree of each node (they are the same number for every node). Unfortunately, I can increase by isotropic diffusion. We consider that this effect is a superficial organization of flow networks. In order to eliminate the effect we subtract it from I. If each flow increases by ϵ with probability $\frac{1}{2}$ and decreases by ϵ with the same probability independently at each step, where ϵ is a uniform random number in $[0, 2\eta]$ then we can easily show that the expected value of increase in I per one step is approximately

$$\frac{2}{3\langle t \rangle} \langle \frac{1}{t} \rangle \eta^2.$$

We define γ by

$$\gamma(0) = \beta(0), \ \gamma(\tau + 1) = \gamma(\tau) + \frac{2}{3\langle t \rangle_\tau} \langle \frac{1}{t} \rangle_\tau \eta^2$$

where $\beta(\tau) = I_\tau - \log \frac{N}{m} = \langle \frac{t}{\langle t \rangle_\tau} \log \frac{t}{\langle t \rangle_\tau} \rangle_\tau$ and $\langle \cdots \rangle_\tau$ denotes average with respect to the distribution of flows at τth period. Note that $\log \frac{N}{m}$ is a constant.

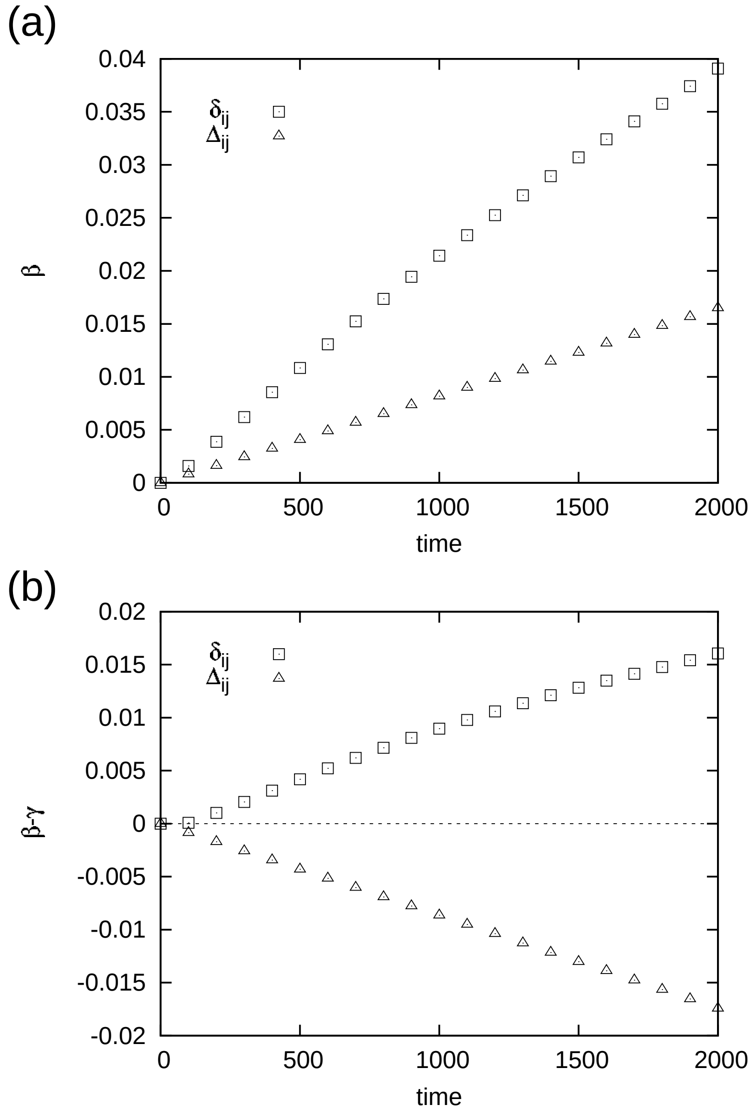

Figure 6.4: (a)Time evolution of β. (b)Time evolution of $\beta - \gamma$.

Figure 6.4 shows the result of our computer simulation averaged over 1000 trials. β increases due to the effect of isotropic diffusion even in the case of Δ_{ij} (Figure 6.4 (a)). However, if the expected value of increase by the effect of isotropic diffusion is subtracted from β then $\beta - \gamma$ increases in the case of δ_{ij} as before on one hand, it decreases in the case of Δ_{ij} on the other hand (Figure 6.4 (b)). This result suggests that if balancing process proceeds by δ_{ij} then flow networks really develop to more organized direction.

Let us examine how flow networks are organized by balancing process. Figure 6.5 (a) shows frequency distribution of flow size in 100 steps from 1000th period accumulated over 1000 trials. In the case of Δ_{ij} the distribution is bell-shaped. On the other hand, the distribution corresponding to δ_{ij} has a long tail toward large flow size. Figure 6.5 (b) shows probability of increase at each flow size estimated from the same data in Figure 6.5 (a). In the case of Δ_{ij} the smaller flow size is, the larger the probability of increase is below mean flow size and the larger flow size is, the smaller the probability of increase is above mean flow size. On the other hand, in the case of δ_{ij} the larger flow size is, the larger the probability of increase is even above mean flow size. Thus flow networks developing by balancing process with δ_{ij} have a self-organizing property that larger flows tend to increase more frequently, which could be seen as a primitive objective. This self-organizing property can generate a distribution of flow size with longer tail. We note that the distributions of flow size of real ecosystems are close to power law distributions that have long tails [107].

In the next section we analyze the mechanism how the results in this section arises through balancing process. In particular, we will see that the self-organizing property that larger flows tend to increase more frequently remains if α is in a sufficiently small neighborhood of $\frac{1}{2}$. This implies that the self-organizing property is robust under small perturbations to α at $\alpha = \frac{1}{2}$.

6.6 Mechanism of Balancing Process

First we see how the behavior of flow networks changes if α is diffrent from $\alpha = \frac{1}{2}$. Figure 6.6 shows that how mean flow size after 2000 periods depends on α. All the other conditions in computer simulation are the same as those in the previous section. It takes maximal values as a function of α at two points $\alpha = 0.4984, 0.5016$, slightly displaced from $\alpha = \frac{1}{2}$. There is a flat region around $\alpha = \frac{1}{2}$ between the two maximal points. As α becomes close to 0 or 1, increase in mean flow size after 2000 periods tends to become 0. Figure 6.7 (a) shows that flow size distributions for $\alpha = 0.5, 0.499, 0.4984$. The distribution for $\alpha = 0.499$ is similar to that for $\alpha = 0.5$ with a long tail toward larger flow size. On the other hand, the distribution for $\alpha = 0.4984$ is a bimodal distribution. Figure 6.7 (b) shows that probability of increase at each flow size. One might expect that organizing mechanisms at $\alpha = 0.4984$ is totally different from that around $\alpha = 0.5$. In order to explain such behaviors next we investigate the mechanism of balancing process.

Since the direction of change of T_{ij} is dependent on four values T_{*i}, T_{i*}, T_{*j}

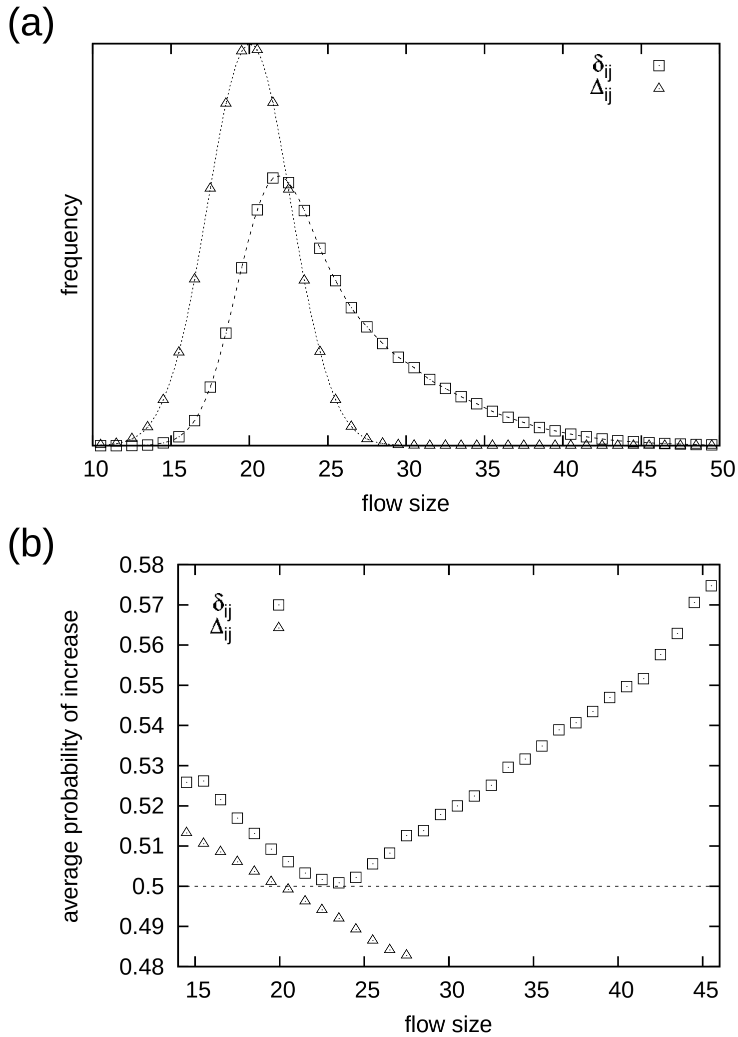

Figure 6.5: (a)Frequency distribution of flow size in 100 steps from 1000th period. (b)Probability of increase at each flow size estimated from the same data in (a).

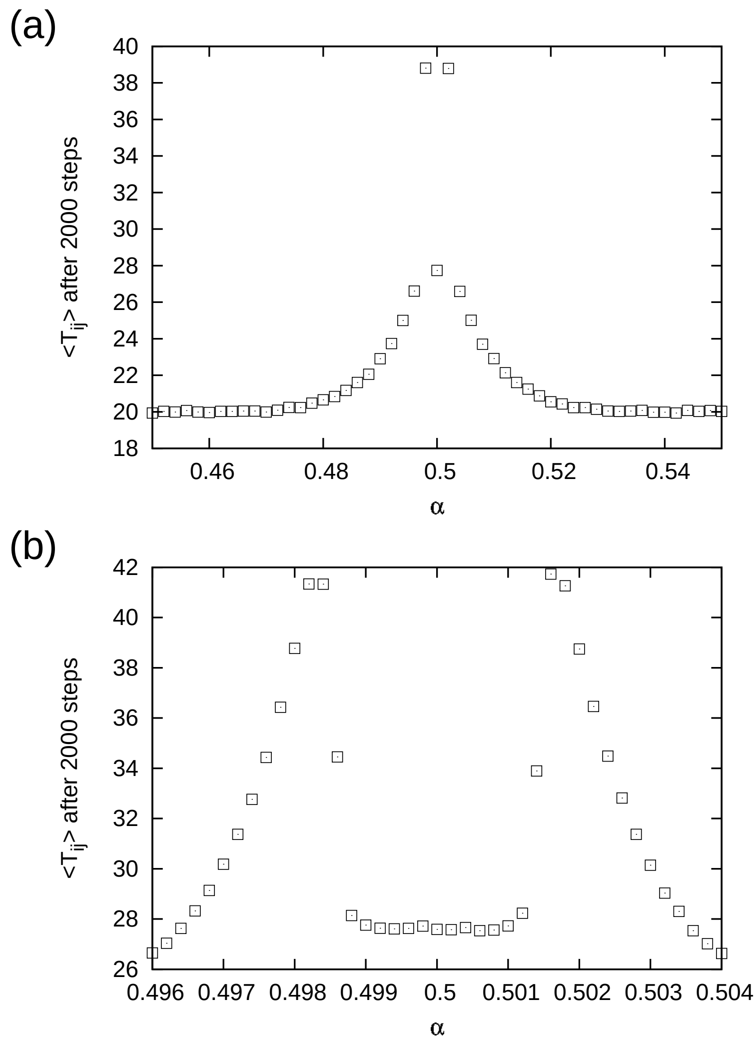

Figure 6.6: (a)Mean flow size after 2000 periods. (b)A magnified picture of (a) around $\alpha = \frac{1}{2}$.

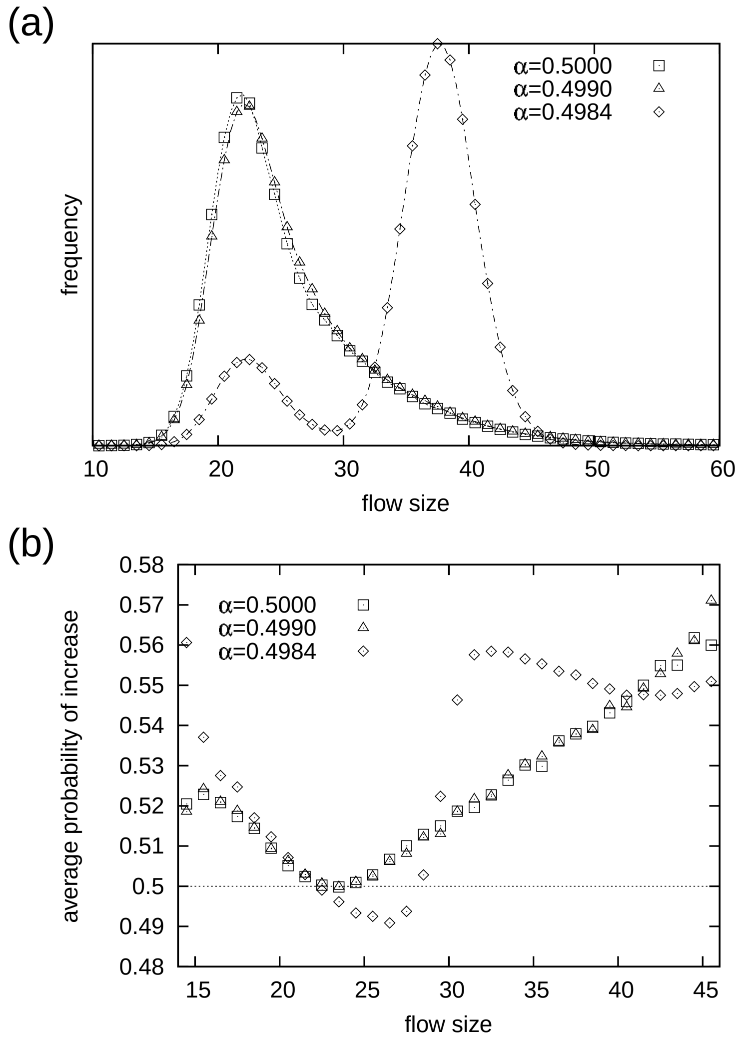

Figure 6.7: (a)Frequency distribution of flow size in 100 steps from 1000th period for $\alpha = 0.5,\ 0.499,\ 0.4984$. (b)Probability of increase at each flow size estimated from the same data in (a).

and T_{j*} we first focus on the relationships between them. We assume that all the four values have different values and all flows with positive sizes also have different values. It is enough to consider $\alpha \leq \frac{1}{2}$ by symmetry.

(i) $T_{*i} > T_{i*}$ **and** $T_{*j} < T_{j*}$**.**

In this case we have

$$\frac{\partial \delta_{ij}}{\partial T_{ij}} = -\alpha \frac{T_{*i}}{T_{i*}^2} - (1-\alpha)\frac{T_{j*}}{T_{*j}^2} < 0.$$

Thus T_{ij} always increases regardless of α.

(ii) $T_{*i} < T_{i*}$ **and** $T_{*j} > T_{j*}$**.**

In this case we have

$$\frac{\partial \delta_{ij}}{\partial T_{ij}} = \alpha \frac{T_{*i}}{T_{i*}^2} + (1-\alpha)\frac{T_{j*}}{T_{*j}^2} > 0.$$

Thus T_{ij} always decreases independent of α.

We can prove that the number of pairs (i,j) that satisfy (i) is the same as the number of pairs (i,j) that satisfy (ii). Indeed, we can assume that $T_{*i} > T_{i*}$ for $1 \leq i \leq n$ and $T_{*i} < T_{i*}$ for $n+1 \leq i \leq N$. Suppose the number of pairs (i,j) with $T_{*i} > T_{i*},\ T_{*j} < T_{j*}$ is k. Then the number of pairs (i,j) with $T_{*i} > T_{i*},\ T_{*j} > T_{j*}$ is $nm-k$. In order to obtain the number of pairs (i,j) with $T_{*i} < T_{i*},\ T_{*j} > T_{j*}$ we subtract the number of pairs (i,j) with $T_{*i} > T_{i*},\ T_{*j} > T_{j*}$ from the number of pairs (i,j) with $T_{*j} > T_{j*}$. That is, the number of pairs (i,j) with $T_{*i} < T_{i*},\ T_{*j} > T_{j*}$ is $nm-(nm-k) = k$. This implies that if two cases (i) and (ii) are combined together then they do not contribute to increase of mean flow size.

(iii) $T_{*i} > T_{i*}$ **and** $T_{*j} > T_{j*}$**.**

Since

$$\frac{\partial \delta_{ij}}{\partial T_{ij}} = -\alpha \frac{T_{*i}}{T_{i*}^2} + (1-\alpha)\frac{T_{j*}}{T_{*j}^2}$$

is a summation of a positive number and a negative number, the sign depends on the relationships between $T_{*i}, T_{i*}, T_{*j}, T_{j*}$ and α.

(iii)-(i) $\frac{T_{i*}}{T_{i*}+T_{*j}} < \alpha$**.**

Since the condition is equivalent to

$$-\alpha \frac{1}{T_{i*}} + (1-\alpha)\frac{1}{T_{*j}} < 0,$$

we obtain

$$\frac{\partial \delta_{ij}}{\partial T_{ij}} = -\alpha \frac{T_{*i}}{T_{i*}^2} + (1-\alpha)\frac{T_{j*}}{T_{*j}^2} < -\alpha \frac{1}{T_{i*}} + (1-\alpha)\frac{1}{T_{*j}} < 0.$$

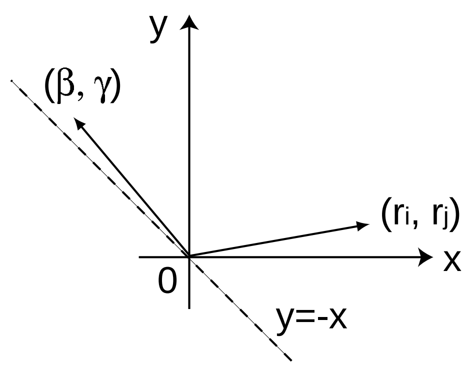

Figure 6.8: $\langle(\beta,\gamma),(r_i,r_j)\rangle$ is negative if the angle between the two vectors is greater than $\frac{\pi}{2}$.

(iii)-(ii) $\alpha < \frac{T_{i*}}{T_{i*}+T_{*j}}$.

Put $r_i = \frac{T_{*i}}{T_{i*}}, r_j = \frac{T_{j*}}{T_{*j}}$. By the condition of (iii), $r_i > 1$ and $r_j < 1$. We also put $\beta = -\alpha\frac{1}{T_{i*}}$ and $\gamma = (1-\alpha)\frac{1}{T_{*j}}$. Then $\frac{\partial\delta_{ij}}{\partial T_{ij}}$ can be represented as an inner product of two plane vectors (β,γ) and (r_i,r_j):

$$\frac{\partial\delta_{ij}}{\partial T_{ij}} = \beta r_i + \gamma r_j = \langle(\beta,\gamma),(r_i,r_j)\rangle,$$

where $\langle\cdots,\cdots\rangle$ is the standard inner product in $\mathbb{R}^2$. Since $\beta < 0,\ \gamma > 0$ and $\beta+\gamma > 0$ by the condition of (iii)-(ii), (β,γ) is in $\{(x,y)\in\mathbb{R}^2 | y > -x,\ x < 0,\ y > 0\}$. On the other hand, since $0 < r_j < 1 < r_i$, (r_i,r_j) is in $\{(x,y)\in\mathbb{R}^2 | y < x,\ x > 0,\ y > 0\}$. Therefore $\langle(\beta,\gamma),(r_i,r_j)\rangle$ tends to be negative if (a) the angle between (β,γ) and $(-1,1)$ is smaller or (b) the angle between (r_i,r_j) and $(1,0)$ is smaller (Figure 6.8). Note that the two conditions (a) and (b) are not independent of each other.

First we consider (a). The closer the inner product

$$\langle(-1,1),\frac{1}{\sqrt{\beta^2+\gamma^2}}(\beta,\gamma)\rangle = \frac{1}{\sqrt{\beta^2+\gamma^2}}(-\beta+\gamma)$$

is to $\sqrt{2}$, the smaller the angle between (β,γ) and $(-1,1)$. In order to see how the value of the inner product depends on T_{ij}, let us assume that $a = \sum_{k\neq j} T_{ik}$ and $b = \sum_{k\neq i} T_{kj}$ are constant and consider the following function.

$$f_\alpha(x) = \frac{1}{\sqrt{(\frac{\alpha}{x+a})^2 + (\frac{1-\alpha}{x+b})^2}}(\frac{\alpha}{x+a} + \frac{1-\alpha}{x+b}).$$

The differential of $f_\alpha(x)$ is

$$f'_\alpha(x) = \frac{\alpha(1-\alpha)(a-b)\{(1-\alpha)a - \alpha b + (1-2\alpha)x\}}{\{(1-\alpha)^2(x+a)^2 + \alpha^2(x+b)^2\}^{\frac{3}{2}}}.$$

There is just one point that gives an extreme value of f_α if $\alpha \neq \frac{1}{2}$. We denote it by

$$x_* = \frac{\alpha b - (1-\alpha)a}{1-2\alpha}.$$

By the condition of (iii)-(ii), we have

$$T_{ij} > \frac{\alpha b - (1-\alpha)a}{1-2\alpha} = x_*.$$

Therefore we only consider the range $x > x_*$. In this range $(1-\alpha)a - \alpha b + (1-2\alpha)x$ is always positive. So the sign of f'_α only depends on $a-b$. If $a > b$ which is equivalent to $T_{i*} > T_{*j}$ then $f_\alpha(x)$ is increasing for $x > x_*$. $f_\alpha(x)$ converges to $\frac{1}{\sqrt{\alpha^2+(1-\alpha)^2}}$ from below as $x \to \infty$. Note that x_* is negative if $a > b$. If $a < b$ which is equivalent to $T_{i*} < T_{*j}$ then $f_\alpha(x)$ is decreasing for $x < x_*$. $f_\alpha(x)$ converges to $\frac{1}{\sqrt{\alpha^2+(1-\alpha)^2}}$ from above as $x \to \infty$. If $\alpha = \frac{1}{2}$ then $f'_\alpha(x)$ has no zero point. Since the condition of (iii)-(ii) becomes $a > b$, $f_\alpha(x)$ is increasing for all $x \in \mathbb{R}$. It converges to $\sqrt{2}$ as $x \to \infty$. However, we can virtually suppose that $f_\alpha(x)$ takes a minimal value at $-\infty$ and treat both cases $\alpha < \frac{1}{2}$ and $\alpha = \frac{1}{2}$ at the same time.

Next we consider (b). The closer the inner product

$$\langle (1,0), \frac{1}{\sqrt{r_i^2 + r_j^2}}(r_i, r_j)\rangle = \frac{r_i}{\sqrt{r_i^2 + r_j^2}}$$

is to 1, the smaller the angle between $(1,0)$ and (r_i, r_j) is. Assuming $p = T_{*i},\ q = T_{j*}$ are constants, we define a function

$$g(x) = \frac{\frac{p}{x+a}}{\sqrt{(\frac{p}{x+a})^2 + (\frac{q}{x+b})^2}}.$$

Since $g(x)$ can be rewritten as

$$g(x) = \frac{1}{\sqrt{1 + (\frac{q}{p})^2(1 + \frac{a-b}{x+b})^2}},$$

$g(x)$ is increasing if $a > b$ and converges to $\frac{1}{\sqrt{1+(\frac{q}{p})^2}}$ from below as $x \to \infty$. If $a < b$ then $g(x)$ is decreasing and converges to $\frac{1}{\sqrt{1+(\frac{q}{p})^2}}$ from above as $x \to \infty$.

Combining both (a) and (b), we can conclude as follows for given $0 \le \alpha \le \frac{1}{2}$. If $T_{i*} > T_{*j}$ then $\frac{\partial \delta_{ij}}{\partial T_{ij}}$ becomes negative more often for larger T_{ij}. If $T_{i*} < T_{*j}$ then $\frac{\partial \delta_{ij}}{\partial T_{ij}}$ becomes negative more often for smaller T_{ij}.

Next we examine how the degrees of the above properties change if α changes. The partial differential of f_α with respect to α is

$$\frac{\partial f_\alpha}{\partial \alpha} = \frac{(x+a)(x+b)\{(1-\alpha)a - \alpha b + (1-2\alpha)x\}}{\{(1-\alpha)^2(x+a)^2 + \alpha^2(x+b)^2\}^{\frac{3}{2}}}.$$

By the condition of (iii)-(ii), $(1-\alpha)a - \alpha b + (1-2\alpha)x$ is always positive hence $\frac{\partial f_\alpha}{\partial \alpha} > 0$. Therefore if α becomes smaller then $f_\alpha(x)$ decreases for a fixed x, which implies that $\frac{\partial \delta_{ij}}{\partial T_{ij}}$ becomes negative less often.

(iv) $T_{*i} < T_{i*}$ and $T_{*j} < T_{j*}$.

In this case we have

$$\frac{\partial \delta_{ij}}{\partial T_{ij}} = -\alpha \frac{T_{*i}}{T_{i*}^2} + (1-\alpha)\frac{T_{j*}}{T_{*j}^2}.$$

So the sign is dependent on $T_{*i}, T_{i*}, T_{*j}, T_{j*}$ and α as in (iii).

(iv)-(i) $\alpha < \frac{T_{i*}}{T_{i*}+T_{*j}}$.

By the condition, we can obtain $\frac{\partial \delta_{ij}}{\partial T_{ij}} < 0$ as in (iii)-(i).

(iv)-(ii) $\frac{T_{i*}}{T_{i*}+T_{*j}} < \alpha$.

As in (iii)-(ii), we represent $\frac{\partial \delta_{ij}}{\partial T_{ij}}$ by an inner product

$$\frac{\partial \delta_{ij}}{\partial T_{ij}} = \langle (\beta', \gamma'), (r_i, r_j) \rangle,$$

where $r_i = \frac{T_{*i}}{T_{i*}}$, $r_j = \frac{T_{j*}}{T_{*j}}$ and $\beta' = \frac{\alpha}{T_{i*}}$, $\gamma' = \frac{1-\alpha}{T_{*j}}$. By a similar argument, we can see that the inner product tends to be negative if (c) the angle between (β', γ') and $(1, -1)$ is smaller or (d) the angle between (r_i, r_j) and $(0, 1)$ is smaller. We can obtain the same function $f_\alpha(x)$ as in (iii)-(ii) for (c). By the condition of (iv)-(ii), we always have $a < b$ if $0 < \alpha \le \frac{1}{2}$. Therefore, again by the condition of (iv)-(ii), the range of x to be considered is $x < x_*$. In this range $f_\alpha(x)$ is increasing.

For (d), we consider the following inner product

$$\langle (0,1), \frac{1}{\sqrt{r_i^2 + r_j^2}}(r_i, r_j) \rangle = \frac{r_j}{\sqrt{r_i^2 + r_j^2}}.$$

As in (iii)-(ii), we define a function

$$h(x) = \frac{\frac{q}{x+b}}{\sqrt{(\frac{p}{x+a})^2 + (\frac{q}{x+b})^2}} = \frac{1}{\sqrt{1 + (\frac{p}{q})^2 (1 + \frac{b-a}{x+a})^2}}.$$

If $a < b$ then $h(x)$ is increasing and converges to $\frac{1}{\sqrt{(\frac{p}{q})^2+1}}$ from below.

Thus one can see that $\frac{\partial \delta_{ij}}{\partial T_{ij}}$ becomes negative more often as T_{ij} becomes large if (c) and (d) are combined together. Moreover, we have $\frac{\partial f_\alpha}{\partial \alpha} < 0$ by the condition of (iv)-(ii). Hence $f_\alpha(x)$ becomes larger as α becomes smaller, which implies that $\frac{\partial \delta_{ij}}{\partial T_{ij}}$ can become negative more often.

So far we argue the non-statistical structures of balancing process. In particular, we find that in the two cases (iii)-(ii) with $T_{i*} > T_{*j}$ and (iv)-(ii) larger T_{ij} can increase more often. Figure 6.9 shows that these structures are effective to generate longer tail flow size distributions around $\alpha = 0.5$ and a bimodal distribution at $\alpha = 0.4984$. The distributions in the controlled numerical experiments are generated by as follows. First we estimate the probability of increase in the case (iii)-(ii) with $T_{i*} > T_{*j}$, which is denoted by p_1, and the probability of increase in the case (iv)-(ii), which is denoted by p_2, from the uncontrolled numerical experiment for each value of α. Second, in the controlled numerical experiments, if T_{ij} satisfies the conditions of (iii), (iii)-(ii) and $T_{i*} > T_{*j}$ (or the conditions of (iv) and (iv)-(ii)), it increases with probability p_1 (or p_2), regardless of flow size. Thus the structures of balancing process described above which enable larger flows to increase more often are broken.

If α is sufficiently close to $\frac{1}{2}$ then the effect of these structures would not so different from that for $\alpha = \frac{1}{2}$ by the continuity of conditions with respect to α appeared in the above argument. This suggests that the self-organizing property at $\alpha = \frac{1}{2}$ observed in the previous section is robust to small perturbations to α.

There are also statistical effects. For example, suppose T_{*i}, T_{i*}, T_{*j} and T_{j*} have values close to mean. If the condition of (iii) $T_{*i} > T_{i*}$ and $T_{*j} > T_{j*}$ is satisfied then the greater T_{ij} is apart from mean flow size toward larger flow size, the smaller $\sum_{k \neq j} T_{ik}$ is in order $T_{*i} > T_{i*}$ to hold. This implies that $T_{i*} < T_{*j}$ is satisfied more often if T_{ij} larger than mean flow size is larger. In addition, the greater T_{ij} is apart from mean flow size toward smaller flow size, the larger $\sum_{k \neq i} T_{kj}$ is in order $T_{*j} > T_{j*}$ to be satisfied. Hence $T_{i*} < T_{*j}$ is satisfied more often if T_{ij} smaller than mean flow size is smaller. Such an effect would be relevant to frequency distribution of flow size within (iii)-(i) if $\alpha \leq \frac{1}{2}$ is close to $\frac{1}{2}$. The same thing can be said for (iv).

There is another statistical effect what we call the effect of threshold. We see $\frac{T_{i*}}{T_{i*}+T_{*j}}$ as a function of T_{ij}. That is, we consider a function

$$k(x) = \frac{x+a}{2x+a+b} = \frac{1}{2}(1 + \frac{a-b}{2x+a+b}),$$

where $a = \sum_{k \neq j} T_{ik}$ and $b = \sum_{k \neq i} T_{kj}$ are supposed to be constants. If $a > b$ then $k(x) > \frac{1}{2}$ for all $x > 0$. If $a < b$ then $k(x)$ is increasing for $x > 0$ and

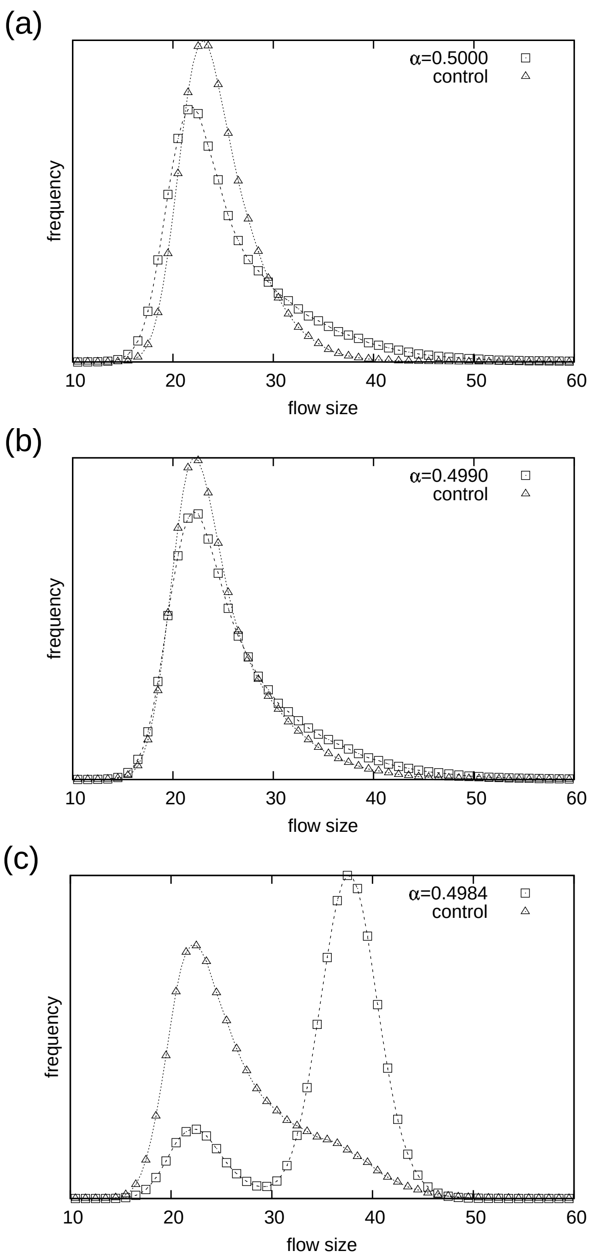

Figure 6.9: Results of controlled numerical experiments in which the structures of balancing process which enable larger T_{ij} to increase more often are broken. See text for details. (a)For $\alpha = 0.5$, $p_1 = 0.035451$ and $p_2 = 0.035566$. (b)For $\alpha = 0.4990$, $p_1 = 0.008836$ and $p_2 = 0.033590$. (c)For $\alpha = 0.4984$, $p_1 = 0.002520$ and $p_2 = 0.004638$.

converges to $\frac{1}{2}$ as $x \to \infty$. Therefore $\alpha < \frac{T_{i*}}{T_{i*}+T_{*j}}$ will be satisfied if T_{ij} is larger than certain threshold value when $\alpha < \frac{1}{2}$. If α is too close to or too far from $\frac{1}{2}$ then such an effect would not be relevant. However, for some values of α the effect of threshold might be significant. For example, the bimodal distribution without long tail for $\alpha = 0.4984$ shown in Figure 6.7 (a) would be a cooperative effect of the effect of threshold and the mechanism for (iii)-(ii) with $T_{i*} < T_{*j}$.

6.7 Conclusions

We give up the position where one can assume macroscopic objectives to which ecosystems organize themselves. At this position we cannot address the relationship between flow balance and macroscopic objectives. Instead, in this chapter we directly describe a dynamics of balancing process and argue how a self-organizing property can arise from the balancing process. Balancing process we proposed is a process of local elimination of imbalances. Since the process of balancing is local, an effort of eliminating an imbalance can lead to generation of new imbalance. As a result of such a process, flow networks can have a self-organizing property.

Objectives are related to wholeness of biological systems. Apparently objectives are unique to biological systems since they seem not to be in physical or chemical systems. However, if one can set an objective that can be identified from the outside of a system then he treats the system as a machine. Any machine is made for certain objective. If it is broken then it is not a machine since it does not have functions that are expected. A broken machine is not a machine, however, it is at least some material. If this material could acquire new functions by itself then we might recognize it as a new machine. Probably one would feel that it is not appropriate to call it machine anymore. In such a situation one would not find a machine but a life. At this point we focus on a system that comes into existence as the system. When a system is recognized as the system, there is already a wholeness that enable the system to come into existence. We call such a wholeness intrinsic wholeness, which is distinguished from a wholeness specified by a macroscopic objective.

In this chapter we attempt to represent intrinsic wholeness as balancing process toward flow balance. Intrinsic wholeness itself does not imply any macroscopic objective, however, balancing process, an effort to maintain intrinsic wholeness, can generates a self-organizing property, which could be seen as a primitive objective.

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