Multimodal Networks: Structure and Operations

Lenwood S. Heath and Allan A. Sioson

Abstract—A multimodal network (MMN) is a novel graph-theoretic formalism designed to capture the structure of biological networks and to represent relationships derived from multiple biological databases. MMNs generalize the standard notions of graphs and hypergraphs, which are the bases of current diagrammatic representations of biological phenomena and incorporate the concept of *mode*. Each vertex of an MMN is a biological entity, a *biot*, while each modal hyperedge is a typed relationship, where the type is given by the mode of the hyperedge. The current paper defines MMNs and concentrates on the structural aspects of MMNs. A companion paper develops MMNs as a representation of the semantics of biological networks and discusses applications of the MMNs in managing complex biological data. The MMN model has been implemented in a database system containing multiple kinds of biological networks.

Index Terms—Multimodal network, graph, hypergraph, biological networks, mode, biot.

1 Introduction

Graphs and hypergraphs are often employed, formally, or informally, to model biological phenomena. The semantics of biological networks are added to these graph-theoretic constructs by labeling vertices, edges, or hyperedges. For example, Pirson et al. [1] propose a methodology to graphically depict biological regulatory information as networks, while Fukuda and Takagi [2] present a method to represent signal transduction pathways using compound graphs.

However, the mere application of a graphical notation for a biological phenomena is only partially effective in representing complex biological information. Biological network models are typically developed from the integration of results from multiple sources in the scientific literature. For example, by integrating various published results, Xanthoudakis and Nicholson [3] formulated a model of an apoptosis pathway mediated by heat-shock proteins. In addition to information integration, it can also be advantageous to select subnetworks of a biological network for detailed analysis. For example, Holme et al. [4] and Schuster et al. [5] decompose biochemical networks into subnetworks to facilitate analyses of metabolic pathways. Another desirable manipulation of complex biological networks is projection, a mapping of, say, a hypergraph to a graph before further analysis. For example, Ma and Zeng [6] project the directed hypergraph structure of metabolic networks found in various organisms to simple graphs to analyze their global structure. Using algebraic set operations such as union, intersection, and difference, Forst et al. [7] compare structures of metabolic networks to derive phylogenetic inference. These examples suggest the importance of not only representing complex biological networks but also of providing graph-theoretic operations for their manipulation.

Multimodal networks (MMNs) [8], [9] provide a structurally rich and extensible graph-theoretic formalism that subsumes the structure of graphs and hypergraphs, both undirected and directed. This paper defines the MMN formalism and the mathematical operations that can be performed on MMNs. The application of MMNs in modeling biological networks is briefly discussed. A companion paper develops MMNs as a representation of the semantics of biological networks and discusses the applications of MMNs in managing complex biological data [10]. Sioson [11] implements the MMN model within a PostgreSQL [12] database system that integrates multiple kinds of biological networks. The term "MMN" is used in different contexts by other researchers. In transportation research, the term has been used to describe transportation networks, where the focus of study is how travelers choose among varied modes of transportation [13] and how to model multimodal transportation network routes [14]. In computing systems research, Abrach et al. [15] used the term to describe a multithreaded operating system with an environment suited for flexible and rapid prototyping of wireless sensor networks. That prototyping environment provides all-virtual, all-physical, and hybrid modes of testing diverse applications across heterogeneous platforms, justifying the use of the word *multimodal*.

2 Graphs, Hypergraphs, and Multimodal Networks

An *undirected graph* (or, simply, a *graph*) is a pair of finite sets (V, E), where the elements of V are called *vertices*, and the elements of E are *unordered* pairs of vertices, called *edges*. An edge between vertices u and v is written $e = (u, v) = (v, u)$; we require that $u \neq v$. The *universal set for undirected graphs* is $\mathcal{UG}$, the set of all undirected graphs. A *directed graph* is a pair of finite sets (V, E), where V is a set of vertices as before, and the elements of E are *ordered* pairs of vertices, called *directed edges*. A directed edge from vertex u to vertex v is written $e = \langle u, v \rangle$; for e, its *tail* and *head*, respectively, are u and v, respectively. We require that

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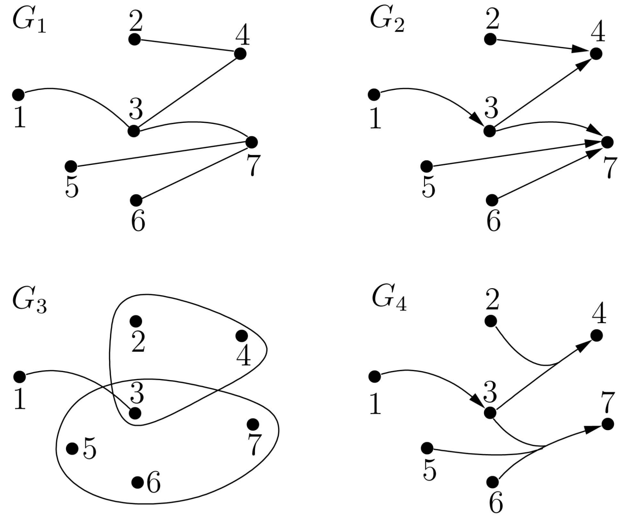

Fig. 1. Drawings of two graph and two hypergraph examples. For all four of these examples, the vertex set is $\{1,2,3,4,5,6,7\}$. G_1 is an undirected graph with edge set $\{(1,3),(2,4),(3,4),\ (3,7),(5,7),(6,7)\}$, while G_2 is a directed graph with edge set $\{\langle 1,3\rangle,\langle 2,4\rangle,\langle 3,4\rangle,$ $\langle 3,7\rangle,\langle 5,7\rangle,\langle 6,7\rangle\}$. G_3 is an undirected hypergraph having hyperedge set $\{\{1,3\},\{2,3,4\},\{3,5,6,7\}\}$ (there are three undirected hyperedges), while G_4 is a directed hypergraph having hyperedge set $\{(\{1\},\{3\}),(\{2,3\},\{4\}),(\{3,5,6\},\{7\})\}$ (there are three directed hyperedges).

$u \neq v$. The *universal set for directed graphs* is $\mathcal{DG}$, the set of all directed graphs. In a drawing of a graph, vertices are dots and edges are curves connecting dots; if the edge is directed, then an arrowhead points to the head of the edge.

An *undirected hypergraph* is a pair of finite sets (V, E), where V is a set of vertices as before and the elements of E are nonempty subsets of V, called *hyperedges* (see Berge [16] for more details). A hyperedge is normally written in set notation such as $\{u, v, w\}$ or $\{x\}$. The *universal set for undirected hypergraphs* is $\mathcal{UH}$, the set of all undirected hypergraphs. A *directed hypergraph* is a pair of finite sets (V, E), where V is a set of vertices as before, and the elements of E are pairs of disjoint subsets of V, called *directed hyperedges* (see Gallo et al. [17] for more details and applications). A directed hyperedge is written as $e = \langle T, H\rangle$, where $T \subseteq V$ is the *tail* of e, and $H \subseteq V$ is the *head* of e. We require that $T \cap H = \emptyset$ and that $T \cup H \neq \emptyset$. The *universal set for directed hypergraphs* is $\mathcal{DH}$, the set of all directed hypergraphs. A hyperedge with more than two vertices is drawn as a closed curve enclosing its vertices. A directed hyperedge is drawn as a merger of a set of arrows connecting each tail vertex to each head vertex. For illustration, see the drawings in Fig. 1.

Undirected and directed hypergraphs are general constructs to model relationships among unrestricted numbers of entities. However, there are representational needs for which neither undirected hypergraphs nor directed hypergraphs are sufficient. First, consider a biochemical example, where a reaction r involving two substrates a and b, in the presence of an enzyme x, results in a product c. In a representation of r, it makes sense to direct edges or hyperedges from a and b (tails) to c (head); however, while x mediates r, it is not a tail; the role of x in r is an *association*. None of the prior representations can cleanly account for these undirected associations, while also accounting for the

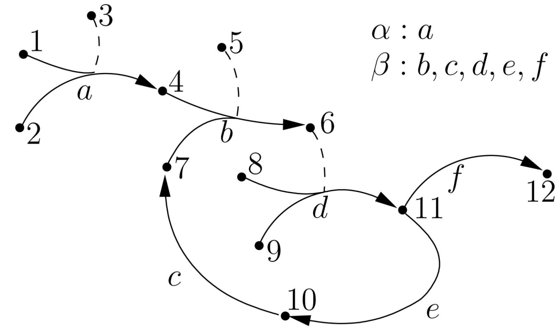

Fig. 2. An example of a MMN N.

clearly directed relationships among entities. To address this need, we bundle heads, tails, and associated entities into a new kind of hyperedge (see below). In the biological literature, most graph-theoretic representations are ad hoc and result in the introduction of one or a small number of mathematical relations tailored to the need at hand. Examples arise in descriptions of biochemical reactions and networks, cellular components, evolution, and implications derived from the experimental literature. To be definite, we use the term *biot* for each of the biological entities that is represented by a vertex in a graph or hypergraph. The combination of multiple relations that involve some common biots results in edges or hyperedges that can be partitioned according to the semantics of the original relations. These relations are *modes* and provide a means of representing both semantics and structure associated with different kinds of biological relations.

An *MMN* is a 3-tuple (V, E, M) of finite sets, where V is a set of vertices as before, each element of E is a 4-tuple from $2^V \times 2^V \times 2^V \times M$, called a *modal hyperedge*, and M is a nonempty set of *modes*. A modal hyperedge $e = (T, H, A, m)$ consists of the *tail* $T \subseteq V$, the *head* $H \subseteq V$, the *associate set* $A \subseteq V$, and a mode $m \in M$. The *empty MMN* is $\Omega = (\emptyset, \emptyset, \emptyset)$. The *universal set for MMNs* is $\mathcal{M}$, the set of all MMNs. When there is no chance of confusion, we simply write hyperedge rather than modal hyperedge (see Fig. 2 for an example of an MMN $N = (V, E, M)$ with vertex set $V = V(N) = \{1,2,3,4,5,6,7,8,9,10,11,12\}$, modal hyperedge set $E = E(N) = \{a, b, c, d, e, f\}$, and mode set $M = M(N) = \{\alpha, \beta\}$. Table 1 lists the six hyperedges).

An MMN is drawn in the same manner as a directed hypergraph with the exception that any associate vertices in a (modal) hyperedge are connected to the merged arrows from tail to head vertices with a dashed curve. In Fig. 2, the hyperedge a has tail $\{1,2\}$, head $\{4\}$, and associate set $\{3\}$;

TABLE 1
The Six Hyperedges of the MMN in Fig. 2

HYPEREDGE	TUPLE
a	$(\{1,2\},\{4\},\{3\},\alpha)$
b	$(\{4,7\},\{6\},\{5\},\beta)$
c	$(\{10\},\{7\},\varnothing,\beta)$
d	$(\{8,9\},\{11\},\{6\},\beta)$
e	$(\{11\},\{10\},\varnothing,\beta)$
f	$(\{11\},\{12\},\varnothing,\beta)$

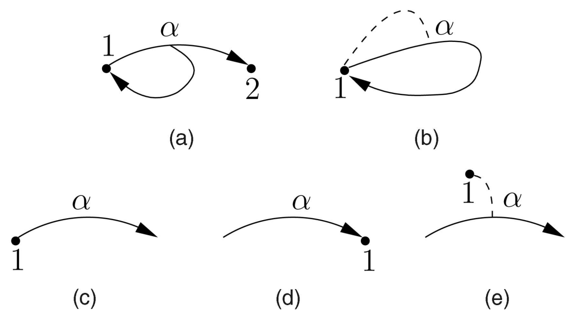

Fig. 3. Five variants on modal hyperedges.

hence, there is direction from 1 and 2 to 4, with a dashed curve from 3. Hyperedge a has mode α, while the remaining hyperedges have mode β; this is indicated at the top of the drawing. Hyperedges b and d are drawn in a similar fashion; note that the head vertex of b is the associate vertex of d. Hyperedges c, e, and f are drawn just as directed edges.

Fix an MMN N, and let $e \in E(N)$. For simplicity in discussing the components of e, we write $T(e)$ for its tail set, $H(e)$ for its head set, $A(e)$ for its associate set, $M(e)$ for its mode, and $V(e) = T(e) \cup H(e) \cup A(e)$ for the set of all of its vertices. For hyperedge a in Fig. 2, we have $T(a) = \{1, 2\}$, $H(a) = \{4\}$, $A(a) = \{3\}$. $M(a) = \alpha$, and $V(a) = \{1, 2, 3, 4\}$.

MMNs constitute a more flexible representational regime for biological networks than previous graph-theoretic formalisms. In addition, the absence of restrictions found in earlier formalisms makes MMNs more mathematically tractable. Here, we list some of the possibilities that the definition of MMNs allows:

1. Two hyperedges in an MMN may have the same tail, head, and associate sets but different modes. For example, the tuple $(\{8, 9\}, \{11\}, \{6\}, \alpha)$ is not identical to the hyperedge d in Fig. 2 and hence could be added to that MMN to obtain an MMN with eight hyperedges.
2. For a hyperedge e, it is possible that $T(e) \cap H(e) \neq \emptyset$, in which case, some arrowheads represent loops at a vertex in $T(e) \cap H(e)$ (see Fig. 3a).
3. For a hyperedge e, it is possible that
$$T(e) \cap H(e) \cap A(e) \neq \emptyset.$$
An example of drawing the hyperedge
$$(\{1\}, \{1\}, \{1\}, \alpha)$$
is found in Fig. 3b.
4. For a hyperedge e, it is possible that two of the three sets $T(e)$, $H(e)$, and $A(e)$ are empty, while the third is not. For example drawings illustrating this, see Fig. 3c, where $e = (\{1\}, \emptyset, \emptyset, \alpha)$; Fig. 3d, where $e = (\emptyset, \{1\}, \emptyset, \alpha)$; and Fig. 3e, where $e = (\emptyset, \emptyset, \{1\}, \alpha)$.
5. For a hyperedge e, it is possible that
$$T(e) = H(e) = A(e) = \emptyset,$$
for example, $e = (\emptyset, \emptyset, \emptyset, \alpha)$. Such hyperedges are not drawn.

Figs. 3a and 3b allows direct modeling of biological networks with special substructures such as feedback mechanisms. For example, Fig. 3a is useful in modeling the biological relationship where a biot, say, gene g, induces the expression of another biot while repressing the expression of itself. A negative feedback regulation mechanism found in *E. coli* illustrates this: the *trp* operon, a set of genes that encode enzymes involved in tryptophan production, is repressed by high quantities of tryptophan [18], [19]. Figs. 3c, 3d, and 3e are useful structures in modeling relationships, where some biots are still unknown or still unidentified.

There are several ways to extend to MMNs those traditional graph-theoretic concepts related to connectivity. The primary issues are the contributions of associated vertices and modes to connectivity. For simplicity and flexibility, we treat each associated vertex of a hyperedge as being available before and after traversing that hyperedge, and we treat modes as not contributing in any way to connectivity (see West [20] for the graph-theoretic terminology that the following is based on).

Let N be an MMN, and let $s, t \in V(N)$. A *walk* $\mathcal{W}$ in N from s to t of length k is an alternating sequence of vertices and hyperedges:

$$v_0, e_1, v_1, \ldots, e_k, v_k,$$

where $s = v_0$, $t = v_k$, and for each j with $1 \leq j \leq k$, we have $v_{j-1} \in T(e_j) \cup A(e_j)$, and $v_j \in H(e_j) \cup A(e_j)$. Vertices s and t are the *source* and *target*, respectively, of $\mathcal{W}$. As an example, for the MMN of that in Fig. 2, the sequence 8, d, 11, e, 10, c, 7, b, 5, b, 6, d, 11 is a walk with source 8, target 11, and length 6. Walk $\mathcal{W}$ is *closed* if $s = t$. Walk $\mathcal{W}$ is a *trail* if it has no repeated hyperedge and is a *cycle* if it is a closed trail such that vertex $s = t$ is the only repeated vertex. Walk $\mathcal{W}$ is a *path* if it has no repeated vertex. Note that a path of length at least 1 is not closed and, hence, is not a cycle. If there exists a path in N with source s and target t, then we say that the path *goes from* s *to* t and that s is *connected* to t.

The previous example walk 8, d, 11, e, 10, c, 7, b, 5, b, 6, d, 11 in the MMN of that in Fig. 2 is not closed and is not a trail, cycle, or path. The walk 1, a, 4, b, 6, d, 11, f, 12 is a trail since it has no repeated hyperedge and is also a path since it has no repeated vertex. The trail 7, b, 6, d, 11, e, 10, c, 7 is a cycle since it is closed (its source and target are both 7) and has no repeated vertex other than 7.

Let

$$v_0, e_1, v_1, \ldots, e_k, v_k,$$

be a walk in N, and let $M' \subseteq M(N)$ be any nonempty subset of the modes of N. $\mathcal{W}$ is an M'-walk in N if, whenever $1 \leq i \leq k$, we have $M(e_i) \in M'$. Again using Fig. 2 for examples, the walk $(1, a, 4, b, 6, d, 11, f, 12)$ is an $\{\alpha, \beta\}$-walk, while the cycle $(7, b, 6, d, 11, e, 10, c, 7)$ is both an $\{\alpha, \beta\}$-walk and a $\{\beta\}$-walk.

3 Mathematical Operations on MMNs

Let $N_1 = (V_1, E_1, M_1)$ and $N_2 = (V_2, E_2, M_2)$ be MMNs. The *union* of N_1 and N_2 is

$$N_1 \cup N_2 = (V_1 \cup V_2,\ E_1 \cup E_2,\ M_1 \cup M_2),$$

while their *intersection* is

$$N_1 \cap N_2 = (V_1 \cap V_2,\ E_1 \cap E_2,\ M_1 \cap M_2).$$

TABLE 2
The Hyperedges of the MMNs N_1 and N_2

HYPEREDGE	TUPLE
a	$(\{1\}, \{2\}, \varnothing, \alpha)$
b	$(\{2,5\}, \{4\}, \varnothing, \beta)$
c	$(\{2,3\}, \{9\}, \{5\}, \beta)$
d	$(\{8,9\}, \{10\}, \varnothing, \beta)$
e	$(\{2,3\}, \{9\}, \{6\}, \beta)$
f	$(\{3,6\}, \{7\}, \varnothing, \beta)$
g	$(\{10\}, \{11\}, \varnothing, \gamma)$
h	$(\{11\}, \{12\}, \varnothing, \gamma)$

Conceptually, the union operation combines the structure and semantics of two MMNs, while the intersection operation isolates their commonalities.

For concreteness, we provide the following example. Let

$$N_1 = (\{1,2,3,4,5,8,9,10\}, \{a,b,c,d\}, \{\alpha,\beta\})$$

and

$$N_2 = (\{2,3,6,7,8,9,10,11,12\}, \{d,e,f,g,h\}, \{\beta,\gamma\})$$

be MMNs, where the hyperedges are given in Table 2. Drawings of N_1 and N_2 can be found in Figs. 4a and 4b. By definition,

$$\begin{aligned} N_1 \cup N_2 = (&\{1,2,3,4,5,6,7,8,9,10,11,12\},\\ &\{a,b,c,d,e,f,g,h\}, \{\alpha,\beta,\gamma\}), \end{aligned}$$

and

$$N_1 \cap N_2 = (\{2,3,8,9,10\}, \{d\}, \{\beta\}).$$

See Figs. 4c and 4d.

Let $N = (V, E, M)$ be an MMN, let $e \in E$, and let u be a new vertex. In particular, $u \notin V$. For $f \in E$, the *contraction* of f by e with u is the hyperedge $g = f \cdot [e, u]$, where

$$\begin{aligned} T(g) &= \begin{cases} T(f) \cup \{u\} \setminus V(e) & \text{if } T(f) \cap V(e) \neq \emptyset, \\ T(f) & \text{otherwise,} \end{cases} \\ H(g) &= \begin{cases} H(f) \cup \{u\} \setminus V(e) & \text{if } H(f) \cap V(e) \neq \emptyset, \\ H(f) & \text{otherwise,} \end{cases} \\ A(g) &= \begin{cases} A(f) \cup \{u\} \setminus V(e) & \text{if } A(f) \cap V(e) \neq \emptyset, \\ A(f) & \text{otherwise,} \end{cases} \\ M(g) &= M(f). \end{aligned}$$

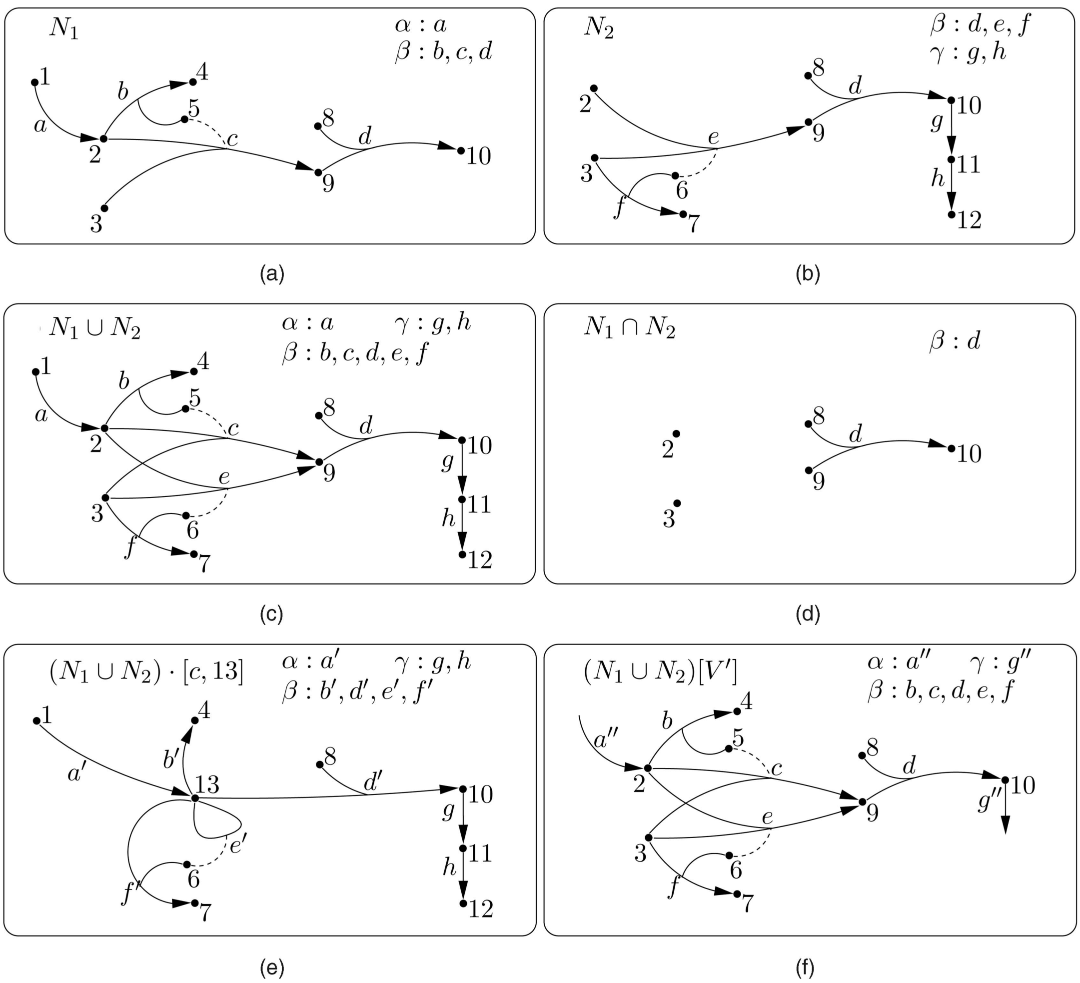

Fig. 4. MMNs N_1 and N_2 and MMN operations. (a) MMN N_1. (b) MMN N_2. (c) Their union. (d) Their intersection. (e) The contraction $N_1 \cup N_2 \cdot [c, 13]$. (f) The subnetwork of $N_1 \cup N_2$ induced by $V' = \{2,3,4,5,6,7,8,9,10\}$.

TABLE 3
Hyperedge Replacements in Fig. 4

Original Hyperedge	Replacement Hyperedge
$a = (\{1\},\{2\},\varnothing,\alpha)$	$a' = a\cdot[c,13] = (\{1\},\{13\},\varnothing,\alpha)$
$b = (\{2,5\},\{4\},\varnothing,\beta)$	$b' = b\cdot[c,13] = (\{13\},\{4\},\varnothing,\beta)$
$d = (\{8,9\},\{10\},\varnothing,\beta)$	$d' = d\cdot[c,13] = (\{8,13\},\{10\},\varnothing,\beta)$
$e = (\{2,3\},\{9\},\{6\},\beta)$	$e' = e\cdot[c,13] = (\{13\},\{13\},\{6\},\beta)$
$f = (\{3,6\},\{7\},\varnothing,\beta)$	$f' = f\cdot[c,13] = (\{13,6\},\{7\},\varnothing,\beta)$

The *contraction* $N\cdot[e,u]$ of e to u in N is

$$\begin{aligned}N\cdot[e,u] =&(V\cup\{u\}\setminus V(e),\{f\cdot[e,u]\mid f\in E\setminus\{e\}\},\\ &\{M(f\cdot[e,u])\mid f\in E\setminus\{e\}\}).\end{aligned}$$

In words, the contraction of e replaces e by the single vertex u and adjusts all remaining hyperedges appropriately. Fig. 4e illustrates the contraction of hyperedge c to new vertex 13 in $N_1\cup N_2$. This contraction $(N_1\cup N_2)\cdot[c,13]$ removes hyperedge c and replaces a number of the remaining hyperedges with new hyperedges, as detailed in Table 3.

Theorem 1. *Let N be an MMN, let e and f be modal hyperedges of N, and let x and y be new vertices. Then, contractions of e and f commute. Precisely, we have that the two double contractions*

$$\begin{aligned}N_{ef} &= (N\cdot[e,x])\cdot[f\cdot[e,x],y],\\ N_{fe} &= (N\cdot[f,y])\cdot[e\cdot[f,y],x]\end{aligned}$$

are isomorphic and, in fact, identical outside the possibility that x is identified with y in an isomorphism.

Proof. There are two cases, depending on whether $V(e)\cap V(f)=\emptyset$ or $V(e)\cap V(f)\neq\emptyset$.

Case 1. $V(e)\cap V(f)=\emptyset$. In both N_{ef} and N_{fe}, we have that each vertex in $V(e)$ maps to x, each vertex in $V(f)$ maps to y, and each vertex in $V(N)\setminus(V(e)\cup V(f))$ maps to itself, because $V(e)\cap V(f)=\emptyset$. Hence, $V(N_{ef})=V(N_{fe})$.

Let $c\in E(N)$ and consider various possibilities for $V(c)$. First, assume that $V(c)\cap V(e)=\emptyset$ and $V(c)\cap V(f)=\emptyset$. Then, by definition of hyperedge contraction, we have that

$$(c\cdot[e,x])\cdot[f\cdot[e,x],y]=(c\cdot[f,y])\cdot[e\cdot[f,y],x]=c.$$

Henceforth, assume that $V(c)\cap V(e)\neq\emptyset$ or $V(c)\cap V(f)\neq\emptyset$; without loss of generality, we may assume that $V(c)\cap V(e)\neq\emptyset$. Consider first the possibility that $V(c)\cap V(f)=\emptyset$. Then, by definition of hyperedge contraction, we have that

$$(c\cdot[e,x])\cdot[f\cdot[e,x],y]=(c\cdot[f,y])\cdot[e\cdot[f,y],x]=c\cdot[e,x].$$

Finally, consider the possibility that $V(c)\cap V(f)\neq\emptyset$. Let $a=(c\cdot[e,x])\cdot[f\cdot[e,x],y]$ and $b=(c\cdot[f,y])\cdot[e\cdot[f,y],x]$. Clearly, $M(a)=M(b)=M(c)$. Let B ambiguously be T, H, or A. Then, we have

$$\begin{aligned}&B(a)=\\ &\begin{cases}(B(c)\cup\{x,y\})\setminus(V(e)\cup V(f)) & \text{if } B(c)\cap V(e)\neq\emptyset\\ & \text{and } B(c)\cap V(f)\neq\emptyset,\\ B(c)\cup\{x\}\setminus V(e) & \text{if } B(c)\cap V(e)\neq\emptyset\\ & \text{and } B(c)\cap V(f)=\emptyset,\\ B(c)\cup\{y\}\setminus V(f) & \text{if } B(c)\cap V(e)=\emptyset\\ & \text{and } B(c)\cap V(f)\neq\emptyset,\\ B(c) & \text{otherwise}\end{cases}\\ &=B(b).\end{aligned}$$

We conclude that $a=b$.

Hence, every hyperedge of N maps to the same hyperedge in both N_{ef} and N_{fe}. We conclude that $M(N_{ef})=M(N_{fe})$ and, indeed, $N_{ef}=N_{fe}$, which establishes the conclusion of the theorem in this case.

Case 2. $V(e)\cap V(f)\neq\emptyset$. In both N_{ef} and N_{fe}, we have that each vertex in $V(N)\setminus(V(e)\cup V(f))$ maps to itself. Since $V(e)\cap V(f)\neq\emptyset$, each vertex in $V(e)\cap V(f)$ maps to x in N_{ef} and to y in N_{fe}. Hence, $V(N_{ef})\setminus V(N_{fe})=\{x\}$ and $V(N_{fe})\setminus V(N_{ef})=\{y\}$. In an isomorphism of N_{ef} and N_{fe}, we will identify every vertex in $V(N)\setminus(V(e)\cup V(f))$ with itself and will identify x and y.

Let $c\in E(N)$, and consider various possibilities for $V(c)$, as in Case 1. The possibilities are identical to those in Case 1, except for the possibility that $V(c)\cap V(e)\neq\emptyset$ and $V(c)\cap V(f)\neq\emptyset$. Again, let $a=(c\cdot[e,x])\cdot[f\cdot[e,x],y]$ and $b=(c\cdot[f,y])\cdot[e\cdot[f,y],x]$, and let B ambiguously be T, H, or A. Again, $M(a)=M(b)=M(c)$. Then, we have

$$B(a)=\begin{cases}(B(c)\cup\{y\})\setminus(V(e)\cup V(f)) & \text{if } B(c)\cap(V(e)\\ & \cup V(f))\neq\emptyset,\\ B(c) & \text{otherwise,}\end{cases}$$

$$B(b)=\begin{cases}(B(c)\cup\{x\})\setminus(V(e)\cup V(f)) & \text{if } B(c)\cap(V(e)\\ & \cup V(f))\neq\emptyset,\\ B(c) & \text{otherwise.}\end{cases}$$

We conclude that an isomorphism that identifies x and y also identifies a and b.

Finally, we observe that $M(N_{ef})=M(N_{fe})$, and hence, we conclude that $N_{ef}=N_{fe}$, which establishes the conclusion of the theorem in this case.

The theorem follows. □

Let $N=(V,E,M)$ be an MMN, let $E'\subseteq E$, and let $V'\subseteq V$. The *subnetwork induced* from N by E' is the MMN $N[E']=(V(E'),E',M(E'))$, where

$$V(E') = \bigcup_{e \in E'} V(e)$$
$$M(E') = \bigcup_{e \in E'} \{M(e)\}.$$

For $e \in E$ satisfying $V(e) \cap V' \neq \emptyset$, the *hyperedge induced* from e by V' is

$$e[V'] = (T(e) \cap V', H(e) \cap V', A(e) \cap V', M(e)).$$

The *subnetwork induced* from N by V' is the MMN:

$$N[V'] = \left(V', \bigcup_{\substack{e \in E \\ V(e) \cap V' \neq \emptyset}} \{e[V']\}, \bigcup_{\substack{e \in E \\ V(e) \cap V' \neq \emptyset}} \{M(e)\} \right).$$

The subnetwork $N[E']$, respectively, $N[V']$, is a *subnetwork* of N *selected* by E', respectively, V'. Fig. 4f illustrates the selection of a subnetwork of $N_1 \cup N_2$ by vertex set $V' = \{2, 3, 4, 5, 6, 7, 8, 9, 10\}$. This example demonstrates that the hyperedges in a subnetwork may differ from hyperedges in the original network. Note that $a'' = a[V'] = (\emptyset, \{2\}, \emptyset, \alpha)$ replaces a, while $g'' = g[V'] = (\{10\}, \emptyset, \emptyset, \gamma)$ replaces g. Moreover, the hyperedge $h = (\{11\}, \{12\}, \emptyset, \gamma)$ does not contribute to $(N_1 \cup N_2)[V']$ because $V' \cap V(h) = \emptyset$.

Theorem 2. *For arbitrary N, P, and $Q \in \mathcal{M}$, the following properties hold:*

1. $\Omega \cap N = \Omega$,
2. $\Omega \cup N = N$,
3. $N \cap P = P \cap N$,
4. $N \cup P = P \cup N$,
5. $N \cap (P \cap Q) = (N \cap P) \cap Q$,
6. $N \cup (P \cup Q) = (N \cup P) \cup Q$,
7. $N \cap (P \cup Q) = (N \cap P) \cup (N \cap Q)$, *and*
8. $N \cup (P \cap Q) = (N \cup P) \cap (N \cup Q)$.

Proof. Using the properties of set union and intersection operations, the proof is straightforward. □

By Theorem 2, both $(\mathcal{M}, \cap)$ and $(\mathcal{M}, \cup)$ are abelian semigroups, that is, both algebraic operations on $\mathcal{M}$ are commutative and associative. Furthermore, $(\mathcal{M}, \cup)$ is an abelian monoid, as Ω is an identity element for $\cup$.

4 Projections

In this section, we relate the capabilities of different graph-theoretic formalisms using projections. Recall that $\mathcal{M}$ is the set of all MMNs; $\mathcal{UG}$ is the set of all undirected graphs; $\mathcal{DG}$ is the set of all directed graphs; $\mathcal{UH}$ is the set of all undirected hypergraphs; and $\mathcal{DH}$ is the set of all directed hypergraphs.

Undirected graph projection. $\Phi_{\mathcal{M} \to \mathcal{UG}} : \mathcal{M} \to \mathcal{UG}$ is the function that takes an MMN $N = (V, E, M)$ to the undirected graph $\Phi_{\mathcal{M} \to \mathcal{UG}}(N) = (V, E')$, where

$$E' = \bigcup_{\substack{e \in E \\ u,v \in V(e) \\ u \neq v}} \{(u, v)\}.$$

In words, each hyperedge e in N is replaced in $\Phi_{\mathcal{M} \to \mathcal{UG}}(N)$ by the complete subgraph on $V(e)$. However, information about direction and modes in hyperedges is lost.

Directed graph projection. $\Phi_{\mathcal{M} \to \mathcal{DG}} : \mathcal{M} \to \mathcal{DG}$ is the function that takes an MMN $N = (V, E, M)$ to the directed graph $\Phi_{\mathcal{M} \to \mathcal{DG}}(N) = (V, E')$, where

$$E' = \bigcup_{e \in E} \left(\Big((T(e) \cup A(e)) \times V(e) \Big) \cup \Big(V(e) \times (A(e) \cup H(e)) \Big) \right) \setminus \left(\bigcup_{v \in V(e)} \{\langle v, v \rangle\} \right).$$

In words, each hyperedge e in N maps to a set of directed edges, without self-loops, that have tail vertices of e as tails, head vertices of e as heads, and associate vertices of e as both tails and heads; mode information is lost.

Theorem 3. *Let N be an MMN. Let $N_U = \Phi_{\mathcal{M} \to \mathcal{UG}}(N)$, and let $N_D = \Phi_{\mathcal{M} \to \mathcal{DG}}(N)$. Then, the cardinality of $E(N_U)$ satisfies the bound:*

$$|E(N_U)| \leq \frac{1}{2} \sum_{e \in E(N)} |V(e)|^2 - |V(e)|,$$

while the cardinality of $E(N_D)$ satisfies the bound,

$$|E(N_D)| \leq \sum_{e \in E(N)} \Big(|V(e)|^2 - |V(e)| \Big).$$

Proof. Each hyperedge $e \in E(N)$ maps to the set of undirected edges $S_e \subseteq E(\Phi_{\mathcal{M} \to \mathcal{UG}}(N))$ given by

$$S_e = \bigcup_{\substack{u,v \in V(e) \\ u \neq v}} \{(u, v)\}.$$

Hence,

$$|S_e| = \binom{|V(e)|}{2} = \frac{|V(e)|^2 - |V(e)|}{2}.$$

Since $E(N_U) = \cup_{e \in E} S_e$, we have

$$|E(N_U)| \leq \sum_{e \in E(N)} |S_e| = \frac{1}{2} \sum_{e \in E(N)} |V(e)|^2 - |V(e)|,$$

as desired.

Each hyperedge $e \in E(N)$ maps to the set of directed edges $S_e \subseteq E(\Phi_{\mathcal{M} \to \mathcal{UG}}(N))$ given by

$$S_e = \left(\Big((T(e) \cup A(e)) \times V(e) \Big) \cup \Big(V(e) \times (A(e) \cup H(e)) \Big) \right) \setminus \left(\bigcup_{v \in V(e)} \{\langle v, v \rangle\} \right) \subseteq V(e) \times V(e) \setminus \left(\bigcup_{v \in V(e)} \{\langle v, v \rangle\} \right).$$

Hence,

$$|S_e| \leq |V(e)|^2 - |V(e)|.$$

Since $E(N_D) = \bigcup_{e \in E} S_e$, we have

$$|E(N_D)| \leq \sum_{e \in E(N)} |S_e| = \sum_{e \in E(N)} |V(e)|^2 - |V(e)|,$$

as desired. □

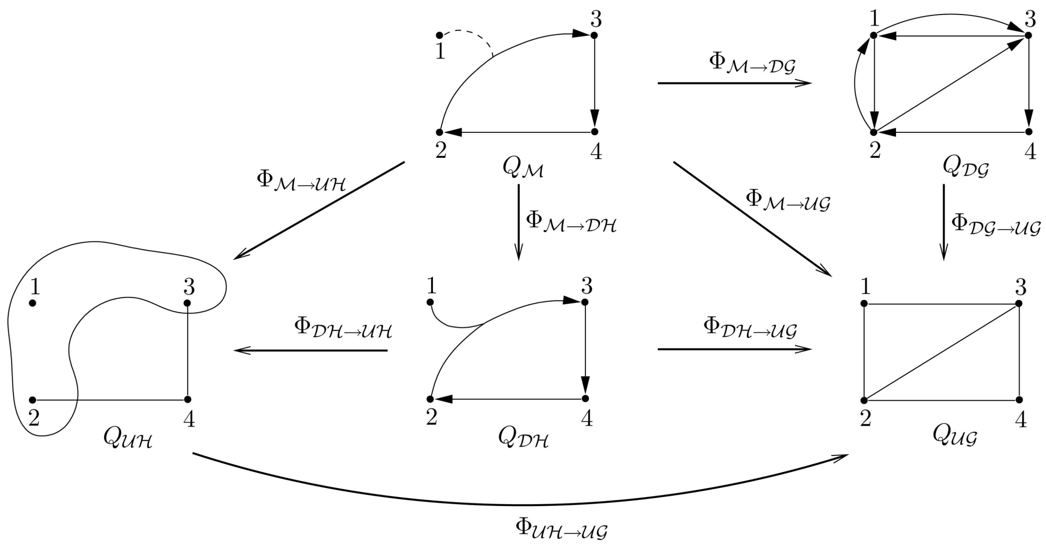

Fig. 5. Projections from one graph-theoretic formalism to another. The MMN $Q_{\mathcal{M}}$ projects to all four other formalisms.

Undirected hypergraph projection. $\Phi_{\mathcal{M}\to\mathcal{UH}} : \mathcal{M} \to \mathcal{UH}$ is the function that takes an MMN $N = (V, E, M)$ to the undirected hypergraph $\Phi_{\mathcal{M}\to\mathcal{UH}}(N) = (V, E')$, where

$$E' = \{V(e) \mid e \in E\}.$$

In words, each hyperedge e in N is replaced in $\Phi_{\mathcal{M}\to\mathcal{UH}}(N)$ by the undirected hyperedge $V(e)$, its set of vertices. Information about direction and modes in hyperedges is lost.

Directed hypergraph projection. $\Phi_{\mathcal{M}\to\mathcal{DH}} : \mathcal{M} \to \mathcal{DH}$ is the function that takes an MMN $N = (V, E, M)$ to the directed hypergraph $\Phi_{\mathcal{M}\to\mathcal{DH}}(N) = (V, E')$, where

$$E' = \{\langle T(e) \cup A(e), H(e) \setminus (T(e) \cup A(e))\rangle \mid e \in E\}.$$

In words, each hyperedge e in N is replaced in $\Phi_{\mathcal{M}\to\mathcal{DH}}(N)$ by the directed hyperedge from $T(e) \cup A(e)$ to $H(e) \setminus (T(e) \cup A(e))$. This bit of finesse is required as the head and tail of a directed hyperedge must be disjoint sets. Information about direction is mostly preserved, but the modes in hyperedges are lost.

Theorem 4. *Let N be an MMN. Let $N_U = \Phi_{\mathcal{M}\to\mathcal{UH}}(N)$ and $N_D = \Phi_{\mathcal{M}\to\mathcal{DH}}(N)$ be projections of N. Then, the cardinalities of the hyperedge sets satisfy these bounds:*

$$|E(N_U)| \le |E(N)|,$$
$$|E(N_D)| \le |E(N)|,$$

with the possibility that either inequality is strict.

Proof. Each modal hyperedge $e \in E(N)$ maps to exactly one undirected hyperedge in $E(N_U)$ and to exactly one directed hyperedge in $E(N_D)$. Neither hyperedge map is necessarily injective. Hence, the bounds $|E(N_U)| \le |E(N)|$ and $|E(N_D)| \le |E(N)|$ hold, along with the possibilities that $|E(N_U)| < |E(N)|$ and $|E(N_D)| < |E(N)|$. □

Projection of a directed hypergraph to an undirected hypergraph. $\Phi_{\mathcal{DH}\to\mathcal{UH}} : \mathcal{DH} \to \mathcal{UH}$ is the function that takes a directed hypergraph $X = (V, E)$ to the undirected hypergraph $\Phi_{\mathcal{DH}\to\mathcal{UH}}(X) = (V, E')$, where

$$E' = \{T(e) \cup H(e) \mid e \in E\}.$$

In words, each hyperedge e in X is replaced in $\Phi_{\mathcal{DH}\to\mathcal{UH}}(X)$ by the undirected hyperedge $T(e) \cup H(e)$, its set of vertices. Information about direction in hyperedges is lost.

Projection of an undirected hypergraph to an undirected graph. $\Phi_{\mathcal{UH}\to\mathcal{UG}} : \mathcal{UH} \to \mathcal{UG}$ is the function that takes an undirected hypergraph $X = (V, E)$ to the undirected graph $\Phi_{\mathcal{UH}\to\mathcal{UG}}(X) = (V, E')$, where

$$E' = \bigcup_{e \in E} \{(u, v) \mid u, v \in V(e) \text{ and } u \neq v\}.$$

In words, each hyperedge e in X is replaced in $\Phi_{\mathcal{UH}\to\mathcal{UG}}(X)$ by a clique on $V(e)$, its set of vertices.

Projection of a directed hypergraph to an undirected graph. $\Phi_{\mathcal{DH}\to\mathcal{UG}} : \mathcal{DH} \to \mathcal{UG}$ is the function that takes an undirected hypergraph $X = (V, E)$ to the undirected graph $\Phi_{\mathcal{DH}\to\mathcal{UG}}(X) = (V, E')$, where

$$E' = \bigcup_{e \in E} \{(u, v) \mid u, v \in T(e) \cup H(e) \text{ and } u \neq v\}.$$

In words, each hyperedge e in X is replaced in $\Phi_{\mathcal{DH}\to\mathcal{UG}}(X)$ by a clique on $T(e) \cup H(e)$, its set of vertices. The direction of hyperedges is lost.

Projection of a directed graph to an undirected graph. $\Phi_{\mathcal{DG}\to\mathcal{UG}} : \mathcal{DG} \to \mathcal{UG}$ is the function that takes a directed graph $G = (V, E)$ to the undirected graph $\Phi_{\mathcal{DG}\to\mathcal{UG}}(G) = (V, E')$, where

$$E' = \bigcup_{\substack{\langle u,v\rangle \in E \\ u \neq v}} \{(u, v)\}.$$

In words, each directed edge e in G is replaced in $\Phi_{\mathcal{DG}\to\mathcal{UG}}(G)$ by an undirected edge between its head and tail. Edge direction is lost.

Fig. 5 illustrates the projections we have defined. Let $Q_{\mathcal{M}}$ be the MMN with

$$\begin{aligned} V(Q_{\mathcal{M}}) = \{1, 2, 3, 4\}, E(Q_{\mathcal{M}}) \\ = \{(\{2\}, \{3\}, \{1\}, \alpha), (\{3\}, \{4\}, \emptyset, \alpha), (\{4\}, \{2\}, \emptyset, \alpha)\}, \end{aligned}$$

and $M(Q_{\mathcal{M}}) = \{\alpha\}$. By definition, projections from $Q_{\mathcal{M}}$ yield these four edge sets:

$$\begin{aligned}
E(\Phi_{\mathcal{M}\to\mathcal{UH}}(Q_{\mathcal{M}})) &= E(Q_{\mathcal{UH}}) \\
&= \{\{1,2,3\},\{3,4\},\{4,2\}\} \\
E(\Phi_{\mathcal{M}\to\mathcal{DH}}(Q_{\mathcal{M}})) &= E(Q_{\mathcal{DH}}) \\
&= \{\langle\{1,2\},\{3\}\rangle,\langle\{3\},\{4\}\rangle,\langle\{4\},\{2\}\rangle\} \\
E(\Phi_{\mathcal{M}\to\mathcal{DG}}(Q_{\mathcal{M}})) &= E(Q_{\mathcal{DG}}) \\
&= \{\langle 2,3\rangle,\langle 2,1\rangle,\langle 1,2\rangle,\langle 3,1\rangle, \\
&\quad \langle 1,3\rangle,\langle 3,4\rangle,\langle 4,2\rangle\} \\
E(\Phi_{\mathcal{M}\to\mathcal{UG}}(Q_{\mathcal{M}})) &= E(Q_{\mathcal{UG}}) \\
&= \{(2,3),(2,1),(3,1),(3,4),(4,2)\}.
\end{aligned}$$

In addition, projection from $Q_{\mathcal{DH}}$ yields the same results as the direct projections from $Q_{\mathcal{M}}$:

$$\begin{aligned}
\Phi_{\mathcal{DH}\to\mathcal{UH}}(Q_{\mathcal{DH}}) &= Q_{\mathcal{UH}}, \\
\Phi_{\mathcal{DH}\to\mathcal{UG}}(Q_{\mathcal{DH}}) &= Q_{\mathcal{UG}}.
\end{aligned}$$

We also have that

$$\begin{aligned}
\Phi_{\mathcal{DG}\to\mathcal{UG}}(Q_{\mathcal{DG}}) &= Q_{\mathcal{UG}}, \\
\Phi_{\mathcal{UH}\to\mathcal{UG}}(Q_{\mathcal{UH}}) &= Q_{\mathcal{UG}}.
\end{aligned}$$

Hence, the diagram in Fig. 5 is commutative [21].

The following theorem generalizes the observations about the example.

Theorem 5. *The following diagram of projections is commutative.*

$$\begin{tikzcd}
& \mathcal{M} \arrow[r, "\Phi_{\mathcal{M}\to\mathcal{DG}}"] \arrow[dl, "\Phi_{\mathcal{M}\to\mathcal{UH}}"'] \arrow[d, "\Phi_{\mathcal{M}\to\mathcal{DH}}"] \arrow[dr, "\Phi_{\mathcal{M}\to\mathcal{UG}}"] & \mathcal{DG} \arrow[d, "\Phi_{\mathcal{DG}\to\mathcal{UG}}"] \\
\mathcal{UH} \arrow[rr, bend right, "\Phi_{\mathcal{UH}\to\mathcal{UG}}"'] & \mathcal{DH} \arrow[l, "\Phi_{\mathcal{DH}\to\mathcal{UH}}"'] \arrow[r, "\Phi_{\mathcal{DH}\to\mathcal{UG}}"] & \mathcal{UG}
\end{tikzcd}$$

Proof. To prove that the diagram is commutative, it suffices to show these four equalities:

$$\begin{aligned}
\Phi_{\mathcal{M}\to\mathcal{UG}} &= \Phi_{\mathcal{DG}\to\mathcal{UG}} \circ \Phi_{\mathcal{M}\to\mathcal{DG}}, \\
\Phi_{\mathcal{M}\to\mathcal{UG}} &= \Phi_{\mathcal{DH}\to\mathcal{UG}} \circ \Phi_{\mathcal{M}\to\mathcal{DH}}, \\
\Phi_{\mathcal{M}\to\mathcal{UH}} &= \Phi_{\mathcal{DH}\to\mathcal{UH}} \circ \Phi_{\mathcal{M}\to\mathcal{DH}}, \\
\Phi_{\mathcal{DH}\to\mathcal{UG}} &= \Phi_{\mathcal{UH}\to\mathcal{UG}} \circ \Phi_{\mathcal{DH}\to\mathcal{UH}}.
\end{aligned}$$

Demonstration that $\Phi_{\mathcal{M}\to\mathcal{UG}} = \Phi_{\mathcal{DG}\to\mathcal{UG}} \circ \Phi_{\mathcal{M}\to\mathcal{DG}}$. Let $N = (V,E,M) \in \mathcal{M}$. By definition of the undirected graph projection of an MMN, $\Phi_{\mathcal{M}\to\mathcal{UG}}(N) = (V,E')$, where

$$E' = \bigcup_{\substack{e\in E \\ u,v\in V(e) \\ u\neq v}} \{(u,v)\}.$$

By definition of the directed graph projection of an MMN, $\Phi_{\mathcal{M}\to\mathcal{DG}}(N) = (V,E'')$, where

$$E'' = \bigcup_{e\in E}(((T(e)\cup A(e))\times V(e))\cup(V(e)\times(A(e)\cup H(e)))) \setminus \left(\bigcup_{v\in V(e)}\{\langle v,v\rangle\}\right).$$

By definition of projection of a directed graph to an undirected graph, $\Phi_{\mathcal{DG}\to\mathcal{UG}}(V,E'')$ has edge set

$$\begin{aligned}
E''' &= \bigcup_{\substack{\langle u,v\rangle\in E'' \\ u\neq v}} \{(u,v)\} \\
&= \bigcup_{e\in E}\left(\bigcup_{\substack{u\in T(e)\cup A(e) \\ v\in V(e) \\ u\neq v}} \{(u,v)\}\right) \bigcup \left(\bigcup_{\substack{u\in V(e) \\ v\in A(e)\cup H(e) \\ u\neq v}} \{(u,v)\}\right) \\
&= \bigcup_{\substack{e\in E \\ u,v\in V(e) \\ u\neq v}} \{(u,v)\} \\
&= E'.
\end{aligned}$$

Hence, $\Phi_{\mathcal{DG}\to\mathcal{UG}}(\Phi_{\mathcal{M}\to\mathcal{DG}}(N)) = \Phi_{\mathcal{M}\to\mathcal{UG}}(N)$, as desired.

Demonstration that $\Phi_{\mathcal{M}\to\mathcal{UG}} = \Phi_{\mathcal{DH}\to\mathcal{UG}} \circ \Phi_{\mathcal{M}\to\mathcal{DH}}$. Let $N = (V,E,M) \in \mathcal{M}$. As before, we have that $\Phi_{\mathcal{M}\to\mathcal{UG}}(N) = (V,E')$, where

$$E' = \bigcup_{\substack{e\in E \\ u,v\in V(e) \\ u\neq v}} \{(u,v)\}.$$

By definition of the directed hypergraph projection of an MMN, $\Phi_{\mathcal{M}\to\mathcal{DH}}(N) = (V,E'')$, where

$$E'' = \{\langle T(e)\cup A(e), H(e)\setminus(T(e)\cup A(e))\rangle \mid e\in E\}.$$

By definition of projection of a directed hypergraph to an undirected graph, the edge set of $\Phi_{\mathcal{DH}\to\mathcal{UG}}(V,E'')$ is

$$\begin{aligned}
E''' &= \bigcup_{\substack{e\in E'' \\ u,v\in T(e)\cup H(e) \\ u\neq v}} \{(u,v)\} \\
&= \bigcup_{e\in E}\left(\bigcup_{\substack{u\in T(e)\cup A(e) \\ v\in H(e)\setminus(T(e)\cup A(e)) \\ u\neq v}} \{(u,v)\}\right) \\
&= \bigcup_{\substack{e\in E \\ u,v\in V(e) \\ u\neq v}} \{(u,v)\} \\
&= E'.
\end{aligned}$$

Hence, $\Phi_{\mathcal{DH}\to\mathcal{UG}}(\Phi_{\mathcal{M}\to\mathcal{DH}}(N)) = \Phi_{\mathcal{M}\to\mathcal{UG}}(N)$, as desired.

Demonstration that $\Phi_{\mathcal{M}\to\mathcal{UH}} = \Phi_{\mathcal{DH}\to\mathcal{UH}} \circ \Phi_{\mathcal{M}\to\mathcal{DH}}$. Let $N = (V,E,M) \in \mathcal{M}$. By definition of the undirected hypergraph projection of an MMN, we have that $\Phi_{\mathcal{M}\to\mathcal{UH}}(N) = (V,E')$, where

$$E' = \{V(e) \mid e\in E\}.$$

By definition of the directed hypergraph projection of an MMN, $\Phi_{\mathcal{M}\to\mathcal{DH}}(N) = (V,E'')$, where

$$E'' = \{\langle(T(e)\cup A(e), H(e))\setminus((T(e)\cup A(e)))\rangle \mid e\in E\}.$$

By definition of projection of a directed hypergraph to an undirected hypergraph, the edge set of $\Phi_{\mathcal{DH}\to\mathcal{UH}}(V, E'')$ is

$$\begin{aligned} E''' &= \{T(e') \cup H(e') \mid e' \in E''\} \\ &= \{(T(e) \cup A(e)) \cup (H(e) \setminus (T(e) \cup A(e)) \mid e \in E\} \\ &= \{V(e) \mid e \in E\} \\ &= E'. \end{aligned}$$

Hence, $\Phi_{\mathcal{DH}\to\mathcal{UH}}(\Phi_{\mathcal{M}\to\mathcal{DH}}(N)) = \Phi_{\mathcal{M}\to\mathcal{UH}}(N)$, as desired.

Demonstration that $\Phi_{\mathcal{DH}\to\mathcal{UG}} = \Phi_{\mathcal{UH}\to\mathcal{UG}} \circ \Phi_{\mathcal{DH}\to\mathcal{UH}}$. Let $X = (V, E) \in \mathcal{DH}$. By definition of the projection of a directed hypergraph to an undirected graph, we have that $\Phi_{\mathcal{DH}\to\mathcal{UG}}(X) = (V, E')$, where

$$E' = \bigcup_{e\in E}\{(u, v) \mid u, v \in T(e) \cup H(e) \text{ and } u \neq v\}.$$

By definition of projection of a directed hypergraph to an undirected hypergraph, the edge set of $\Phi_{\mathcal{DH}\to\mathcal{UH}}(V, E')$ is

$$E'' = \{T(e) \cup H(e) \mid e \in E\}.$$

By definition of projection of an undirected hypergraph to an undirected graph, the edge set of $\Phi_{\mathcal{UH}\to\mathcal{UG}}(V, E'')$ is

$$\begin{aligned} E''' &= \bigcup_{e\in E''}\{(u, v) \mid u, v \in V(e) \text{ and } u \neq v\} \\ &= \bigcup_{e\in E}\{(u, v) \mid u, v \in T(e) \cup H(e) \text{ and } u \neq v\} \\ &= \bigcup_{e\in E}\{(u, v) \mid u, v \in T(e) \cup H(e) \text{ and } u \neq v\} \\ &= E'. \end{aligned}$$

Hence, $\Phi_{\mathcal{UH}\to\mathcal{UG}}(\Phi_{\mathcal{DH}\to\mathcal{UH}}(N)) = \Phi_{\mathcal{DH}\to\mathcal{UG}}(N)$, as desired. $\square$

Theorem 5 suggest that projections preserve some structure as we transform one graph-theoretic formalism into another. A more detailed indication of structure preservation is the path preservation demonstrated in the next theorem.

Theorem 6. *Let N be an MMN, and let $\mathcal{P} = v_0, e_1, v_1, \ldots, e_k, v_k$ be a path of length k in N. Then, the following statements hold:*

1. *There is a path in $\Phi_{\mathcal{M}\to\mathcal{UG}}(N)$ from v_0 to v_k whose vertex sequence is $v_0, v_1, \ldots, v_k$.*
2. *There is a path in $\Phi_{\mathcal{M}\to\mathcal{DG}}(N)$ from v_0 to v_k whose vertex sequence is $v_0, v_1, \ldots, v_k$.*
3. *There is a path in $\Phi_{\mathcal{M}\to\mathcal{UH}}(N)$ from v_0 to v_k whose vertex sequence is $v_0, v_1, \ldots, v_k$.*

Proof. Since $\mathcal{P}$ is a walk, for each j with $1 \leq j \leq k$, we have $v_{j-1} \in T(e_j) \cup A(e_j)$, and $v_j \in H(e_j) \cup A(e_j)$. Since $\mathcal{P}$ is a path, it has no repeated vertices:

1. Consider an edge e_j in $\mathcal{P}$, which implies that v_{j-1}, $v_j \in V(N)$, and $v_{j-1} \neq v_j$. By definition of $\Phi_{\mathcal{M}\to\mathcal{UG}}(N)$, $e'_j = (v_{j-1}, v_j)$ is in the edge set of $\Phi_{\mathcal{M}\to\mathcal{UG}}(N)$. Hence, $v_0, e'_1, v_1, e'_2, v_2, \ldots, e'_k, v_k$ is a path in the undirected graph $\Phi_{\mathcal{M}\to\mathcal{UG}}(N)$, as desired.
2. By definition of the directed graph projection of an MMN, $\Phi_{\mathcal{M}\to\mathcal{DG}}(N) = (V(N), E')$, where
$$E' = \bigcup_{e\in E(N)} ((T(e) \cup A(e)) \times V(e)) \cup (V(e); \times(A(e) \cup H(e))) \setminus \left(\bigcup_{v\in V(e)} \{\langle v, v\rangle\}\right).$$
Consider an edge e_j in $\mathcal{P}$. Since $v_{j-1} \in T(e_j) \cup A(e_j)$, $v_j \in V(e_j)$, and $v_{j-1} \neq v_j$, we have $e'_j = \langle v_{j-1}, v_j\rangle \in E'$. Hence,
$$v_0, e'_1, v_1, e'_2, v_2, \ldots, e'_k, v_k$$
is a path in the directed graph $\Phi_{\mathcal{M}\to\mathcal{DG}}(N)$, as desired.
3. By definition of the undirected hypergraph projection of an MMN, $\Phi_{\mathcal{M}\to\mathcal{UH}}(N) = (V, E')$, where
$$E' = \{V(e) \mid e \in E(N)\}.$$
Consider an edge e_j in $\mathcal{P}$. By the definition, we have $V(e_j) \in E'$. Since v_{j-1}, $v_j \in V(e_j)$ and $v_{j-1} \neq v_j$, we conclude that $v_0, e'_1, v_1, e'_2, v_2, \ldots, e'_k, v_k$ is a path in the undirected hypergraph $\Phi_{\mathcal{M}\to\mathcal{UH}}(N)$, as desired.

$\square$

In contrast to the conclusions of Theorem 6, the existence of a path $\mathcal{P}$ from s to t in an MMN N does not guarantee the existence of a path from s to t in the directed hypergraph $\Phi_{\mathcal{M}\to\mathcal{DH}}(N)$. As a simple example, let

$$N = (\{1, 2, 3, 4\}, \{(\{1, 2\}, \{3\}, \{4\}, \alpha)\}, \{\alpha\}).$$

Then,

$$\Phi_{\mathcal{M}\to\mathcal{DH}}(N) = (\{1, 2, 3, 4\}, \{\langle\{1, 2, 4\}, \{3\}\rangle\}, \{\alpha\}).$$

There is a path $1, (\{1, 2\}, \{3\}, \{4\}, \alpha), 4$ from 1 to 4 in N, but there is no path from 1 to 4 in $\Phi_{\mathcal{M}\to\mathcal{DH}}(N)$.

MMN N is *connected* if, for every pair of vertices s, $t \in V(N)$, there is a path from s to t in $\Phi_{\mathcal{M}\to\mathcal{UG}}(N)$. MMN N is *strongly connected* if, for every pair of vertices $s, t \in V(N)$, there exists a path from s to t in N. Undirected graph G is *connected* if, for every pair of vertices s, $t \in V(G)$, there exists a path from s to t in G. Directed graph G is *strongly connected* if, for every pair of vertices s, $t \in V(G)$, there exists a path from s to t in G. Undirected hypergraph X is *connected* if for every pair of vertices $s, t \in V(X)$, there exists a path from s to t in X. Directed hypergraph X is *strongly connected* if for every pair of vertices $s, t \in V(X)$, there exists a path $\mathcal{P}$ from s to t in X.

Theorem 7. *Let N be a connected MMN. Then, both $\Phi_{\mathcal{M}\to\mathcal{UG}}(N)$ and $\Phi_{\mathcal{M}\to\mathcal{UH}}(N)$ are connected.*

Proof. Let s, $t \in V(N)$. Since N is connected, there exists a path from s to t in N. By Theorem 6, there exists a path from s to t in $\Phi_{\mathcal{M}\to\mathcal{UG}}(N)$. As s and t are arbitrary, it follows that $\Phi_{\mathcal{M}\to\mathcal{UG}}(N)$ is connected.

By an analogous argument, we obtain that $\Phi_{\mathcal{M}\to\mathcal{UH}}(N)$ is connected. $\square$

Theorem 8. *Let N be a strongly connected MMN. Then, $\Phi_{\mathcal{M}\to\mathcal{DG}}(N)$ is strongly connected.*

TABLE 4
Paths in $Q_{\mathcal{M}}$ That Together Demonstrate That $Q_{\mathcal{M}}$ Is Strongly Connected

SOURCE	TARGET	PATH
1	2	$1, a, 3, b, 4, c, 2$
1	3	$1, a, 3$
1	4	$1, a, 3, b, 4$
2	3	$2, a, 3$
2	4	$2, a, 3, b, 4$
3	4	$3, b, 4$
2	1	$2, a, 1$
3	1	$3, b, 4, c, 2, a, 1$
4	1	$4, c, 2, a, 1$
3	2	$3, b, 4, c, 2$
4	2	$4, c, 2$
4	3	$4, c, 2, a, 3$

Proof. Since MMN N is strongly connected, then for every pair of vertices $s,\, t \in V(N)$, there exists a path $\mathcal{P}$ from s to t in N. By Theorem 6, to every path $\mathcal{P}$ from s to t in N, there corresponds a path $\mathcal{P}'$ from s to t in $\Phi_{\mathcal{M}\rightarrow\mathcal{DG}}(N)$. Since $V(N) = V(\Phi_{\mathcal{M}\rightarrow\mathcal{DG}}(N))$, it follows that every pair of vertices $s, t \in V(\Phi_{\mathcal{M}\rightarrow\mathcal{DG}}(N))$, there exists a path $\mathcal{P}'$ from s to t in $\Phi_{\mathcal{M}\rightarrow\mathcal{DG}}(N)$. Hence, $\Phi_{\mathcal{M}\rightarrow\mathcal{DG}}(N)$ is strongly connected. □

In contrast to the conclusion of Theorem 8, the fact that an MMN N is strongly connected does not guarantee that the directed hypergraph $\Phi_{\mathcal{M}\rightarrow\mathcal{DH}}(N)$ is also strongly connected. In Fig. 5, take MMN $Q_{\mathcal{M}}$ and $Q_{\mathcal{DH}} = \Phi_{\mathcal{M}\rightarrow\mathcal{DH}}(Q_{\mathcal{M}})$ as an example. The collection of paths documented in Table 4 demonstrates that MMN $Q_{\mathcal{M}}$ is strongly connected. However, $Q_{\mathcal{DH}}$ is not strongly connected, as it contains no paths from 2 to 1, 3 to 1, or 4 to 1.

5 Modeling Biological Networks

The representation of a biological phenomenon is often given as a network exhibiting multiple types of relationships or interactions of biots (biological entities), drawn in a single diagram. A particular relationship among biots may or may not be binary, while the role of a biot may differ from one relationship to another. This structural richness of biological networks is not readily represented with traditional graph-theoretic formalisms but can be readily represented with the MMN formalism. In an MMN, the vertices are the biots, while the relationships or interactions are modal hyperedges. Different modal hyperedges that uses a particular biot may have different modes, typically representing the different role the biot has in different contexts. Most conveniently, we associate each mode with exactly one type of biological relationship or interaction.

With biological networks represented as MMNs, the union operation can integrate these separate biological networks into a larger MMN. The intersection operation on the other hand allows identification of common interaction structures between two distinct MMNs. An application would be the identification of a common structure of pathways (perhaps conserved structures) between the biological network models of different organisms, say, *Arabidopsis thaliana* and *Saccharomyces cerevisiae*. The subnetwork selection operation is useful in studying a small part of a biological MMN.

The hyperedge contraction is often employed in biological literature and biological databases when representing biological relationships as a single concept. For example, a metabolic pathway is represented as a single biot when discussing its relationship to another pathway. The Kyoto Encyclopedia of Genes and Genomes (KEGG) metabolic pathway database uses a biot to represent the Citrate cycle in its graphical overview of the Glycolysis metabolic pathway, though further detail of the Citrate cycle is available elsewhere in the KEGG pathway database (see the KEGG Web site [22]). Various graph and hypergraph projections of a MMN are applicable if we wish to employ a computational tool that requires a different graph-theoretic formalism as input. For example, while in-silico metabolic networks data from KEGG have directed hypergraph structure, projecting directed graphs from it allowed Ma and Zeng [6] to use standard graph algorithms such as breadth-first search to analyze the global structure of metabolic networks of various organisms.

Fig. 6 is a biological network model based on a pathway proposed by Xanthoudakis and Nicholson [3] to account for the modulation of apoptosis by heat shock proteins. This network model has the structure of MMN $N_1 \cup N_2$ in Fig. 4c. One result they incorporate in their model comes from Bruey et al. [23], who demonstrate that hsp27 negatively regulates cell death through interaction with cytochrome c. Fig. 6 shows that cytochrome c released from mitochondria can either be bound to hsp27 or Apaf-1. Here, hsp27, as an associate, affects negatively the formation of apoptosome (i.e., modal hyperedge e_3). Similarly, Apaf-1 can either bind with hsp70 or with cytochrome c. Hsp70 has been suggested to negatively affect the formation of apoptosome [24], [25]. The apoptosome when bound with caspase-9 causes caspase-3 activation, which then leads to apoptosis. In this MMN model formed by doing a union of inferences modeled as modal hyperedges, hsp70 and hsp27 are shown to modulate cell death.

6 Conclusion

This paper covers the structure and operations on MMNs. When modes are chosen to have biological meaning, it provides a way to understand the semantics of the overall model represented by an MMN. However, the semantics each mode provides is limited to the general structure of a hyperedge. In a related work on MMNs, we use denotational semantics to incorporate computational meaning on the interaction among vertices of each hyperedge. A language that allows specification and simulation of computational semantics on each hyperedge is developed to support this work. Furthermore, we implemented a database prototype that demonstrates how the available biological data such as metabolic pathway data from KEGG [22], [26], [27] and microarray expression data from the Expresso project [28], [29] at the Virginia Polytechnic Institute and State University (Virginia Tech) are modeled as MMNs. We used the PostgreSQL database management

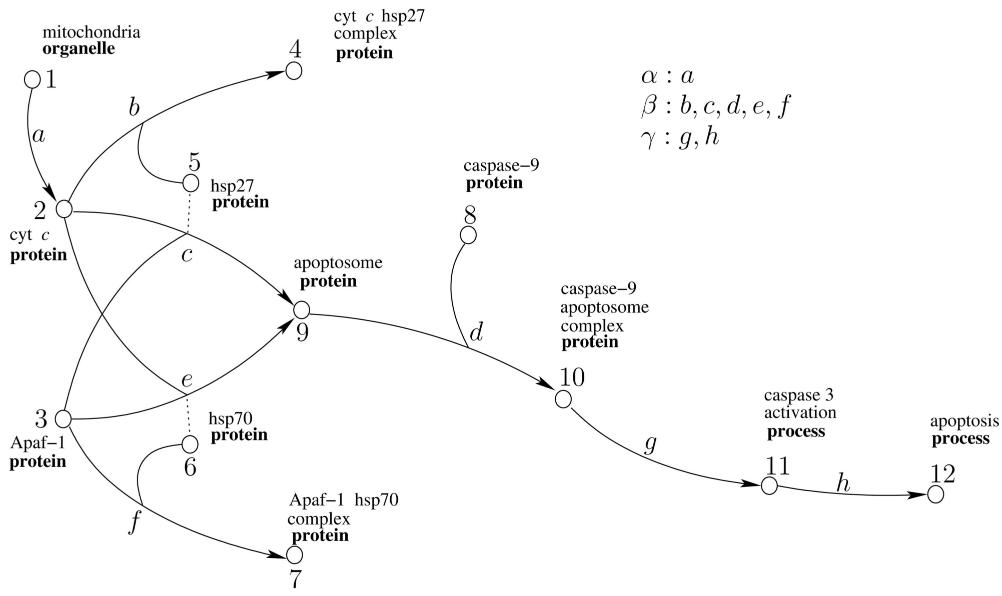

Fig. 6. A biological MMN model. Here, the semantics of the three modes is given by α means "releases," β means "forms complex," γ means "leads to."

system [12] to define the structure of MMNs. In the prototype, the MMN operations and projections are implemented as PostgreSQL database functions using the PL/PgSQL language (see Sioson [11] for details on the implemented MMN prototype).

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