On the computability of atomic subfunctors with applications to cocompletion

Erwan Beurier
Département de Génie Informatique et Génie Logiciel, Polytechnique Montréal
Montréal, Québec, Canada
IRT SystemX
2 boulevard Thomas Gobert, 91120 Palaiseau, France
erwan.beurier@polymtl.ca

Dominique Pastor
Mathematical and Electrical Engineering Department, IMT Atlantique
Brest, France
dominique.pastor@imt-atlantique.fr

Nora Boulahia-Cuppens   Frédéric Cuppens
Département de Génie Informatique et Génie Logiciel, Polytechnique Montréal
Montréal, Québec, Canada
nora.boulahia-cuppens@polymtl.ca   frederic.cuppens@polymtl.ca

This note studies the subfunctors of a given functor F to the category of sets. We provide an algorithm to enumerate all subfunctors of F whose image, for each object, is a singleton. This result applies to the enumeration of clusters, seen as the atomic subfunctors of a functor of connected components. We also use this algorithm in another procedure verifying if the Multiplicity Principle holds.

1 Introduction

In their categorical modelling of biological systems, [8] proposes a mathematical definition of emergence using the property referred to as the Multiplicity Principle (MP). This property is reused later to describe the resilience of systems in categorical terms [11]. The MP is the property of two diagrams to a given category, whose cocones are isomorphic, but such that the isomorphism cannot be written as a composition functor. This composition functor is defined using clusters [8, 5, 6] and it is thus crucial to be able to detect or even enumerate clusters for the MP.

Preliminary work may be found in [5, Part III, Chapter 5, pages 145-172] and [6, Section 3, Proposition 3.4, page 498], dedicated to clusters. In this note, we extend this preliminary work to general atomic subfunctors defined as functors to the category of sets and whose image, for each object, is a singleton. Indeed, clusters are the arrows of a free cocompletion and turn out to be atomic subfunctors of the functor of connected components of the comma-category between two diagrams [6, Section 3, Proposition 3.4, page 498]. We also use describe a procedure to detect the Multiplicity Principle in a computational way.

This question is tackled in an elementary way, as only basic knowledge of category theory is required to follow this note.

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1.1 Notation

Let F be either a function $F : \mathrm{Ob}(\mathscr{C}) \to Sets$ or a functor $F : \mathscr{C} \to Sets$. If U is a function $U : \mathrm{Ob}(\mathscr{C}) \to Sets$, we write $U \subset F$ and say that U is a sunfunction of F when for all $C \in \mathscr{C}$, $U(C) \subset F(C)$. We extend the notation $\subset$ to subfunctors: we write $V \subset F$ when V is a subfunctor of F, that is, when for all $C \in \mathscr{C}$, $V(C) \subset F(C)$, and for all $c : C \to C'$, $V(c) = F(c)|_{V(C)}$. Similarly, if U and V are two functions $\mathrm{Ob}(\mathscr{C}) \to Sets$, we define $U \cap V$ and $U \cup V$ componentwise: $U \cap V : C \mapsto U(C) \cap V(C)$ and $U \cup V : C \mapsto U(C) \cup V(C)$. If $(V_\alpha)_\alpha$ is a sequence of functions $\mathscr{C} \to Sets$, the intersection $\bigcap\limits_\alpha V_\alpha$ and union $\bigcup\limits_\alpha V_\alpha$ are also defined componentwise.

In this note, we consider a fixed functor $F : \mathscr{C} \to Sets$ and a variable function $U : \mathrm{Ob}(\mathscr{C}) \to Sets$ (note that this implies that $\mathscr{C}$ is small). We also use the letter V and X (respectively) as variables for general (resp. atomic) subfunctors of F (definition below).

Besides, when we construct a subfunctor of F, we do not specify the action on arrows, as it will necessarily be the same action as F, on a restricted domain. Thereby, in this note, we define a subfunctor through its action on objects.

2 Preliminaries

It is well-known that a subfunctor V of $F : \mathscr{C} \to Sets$ is determined by a monic natural transformation in $Func(\mathscr{C}, Sets)$ [10, Chapter I, Section 4, pages 35-36] [3, Chapter 4, Section 4.3.14, Exercise 3, page 116] [4, Chapter 1, Section 4, Exercices 1.4, page 22]. Thus, a subfunctor is a function with a certain structure.

As shown in [9, Paragraph 1], and recalled in a more "set-ish" manner in [13, Section 4, pages 362-363], there are two ways to construct a subfunctor (or subpresheaf in the cited sources) of F from a subfunction U. On the one hand, we have the maximal subfunctor contained in U, hereby denoted by $\overline{U}$ given by the following formula:

$$\begin{aligned} \overline{U}(C_0) &= \{x \in F(C_0) \mid \forall c : C_0 \to C, F(c)(x) \in U(C)\} \\ &= \bigcap_{c : C_0 \to C} F(c)^{-1}(U(C)) \end{aligned} \qquad (\star)$$

On the other hand, we have the minimal subfunctor of F containing U, hereby denoted by $\underline{U}$ and defined by the following formula:

$$\begin{aligned} \underline{U}(C_0) &= \{y \in F(C_0) \mid \exists c : C \to C_0, \exists x \in U(C_0), F(c)(x) = y\} \\ &= \bigcup_{c : C \to C_0} F(c)(U(C)) \end{aligned}$$

We recalled the existence of those constructions for the sake of completeness. However, in this note, we consider the former construction only, that of the maximum subfunctor of F contained in U.

By definition of $\overline{U}$, the following result is straightforward but will prove useful in the sequel.

Lemma 2.1. *If $\overline{U}$ is the maximal subfunctor of F contained in U, then the following holds:*

1. *If V is a subfunctor such that $V \subset U \subset F$, then $V \subset \overline{U}$.*
2. *If U is already a subfunctor of F then $U = \overline{U}$.*

The proofs are left to the reader.

3 Enumerating atomic subfunctors

In the following, we present a procedure to enumerate the class of atomic subfunctors, as defined below.

Definition 3.1 (Atomic subfunctor)**.** An *atomic subfunctor of* $F : \mathscr{C} \to Sets$ is a subfunctor $X \subset F$ such that, for all $C \in \mathscr{C}$, $\operatorname{card}(X(C)) = 1$.

Given a function $U \subset F$ and a set of pairs $\mathbb{P} = \{(C, E \in F(C)), \ldots\}$ (this set $\mathbb{P}$ will be called *partial choice* in the following), our procedure EnumerateAtomic$(F, U, \mathbb{P})$ specified in Procedure EnumerateAtomic outputs the set of atomic subfunctors X of F contained in U such that for all $(C, E) \in \mathbb{P}$, $X(C) = \{E\}$. This procedure derives from a series of results formalizing the following heuristic.

Consider the set $\mathbb{P} = \{(C_0, E_0)\}$. We first initialize the algorithm by constructing a copy X of F, except for C_0 that we assign to the singleton $X(C_0) = \{E_0\} \subset F(C_0)$, as constrained by $\mathbb{P}$.

For now, X is a function, and not a functor. We "spread" the choice of $\{E_0\}$ to the rest of the function by constructing the maximal subfunctor $\overline{X}$. Think of this spread as a "spread of functoriality".

If this "spread" results in an empty set for some C, then there is no atomic subfunctor X with $X(C_0) = \{E_0\}$. If the spread finishes with a function X whose components have cardinality 1, then it is an atomic subfunctor and the procedure stops. If the spread stops but the resulting function has some components with cardinality > 1, then we try again as follows. We keep $X(C_0) = \{E_0\}$ as defined in $\mathbb{P}$, and, for some C_1 such that $\operatorname{card}(X(C_1)) > 1$, we try and set $X(C_1) = \{E_1\}$, for some element $E_1 \in X(C_1)$. We "spread" this choice of $\{E_1\}$, again by considering the maximal subfunctor $\overline{X}$. If $\overline{X}$ is empty, then there is no atomic subfunctor X with $X(C_0) = \{E_0\}$ and $X(C_1) = \{E_1\}$, and we try again with another E_1'. If the resulting function has all $X(C)$ with cardinality 1, then X is an atomic subfunctor. If again the resulting X has some components $X(C)$ with cardinality greater than 1, then we repeat the algorithm, this time with three choices, and so on.

In the following, we establish the results needed to prove that the algorithm actually performs as expected.

Lemma 3.2. *If X is a subfunctor of $F : \mathscr{C} \to Sets$ then, for all $C_0 \in \mathscr{C}$:*

$$X(C_0) = \bigcap_{c:C_0 \to C} F(c)^{-1}(X(C))$$

Besides, if X is atomic, then:

$$X(C_0) = \bigcap_{c:C \to C_0} F(c)(X(C))$$

Proof. For the first equality, as X is a subfunctor, for all $c : C_0 \to C$, $F(c)(X(C_0)) \subset X(C)$ hence the direct inclusion $\subset$. Also note that

$$\bigcap_{c:C_0 \to C} F(c)^{-1}(X(C)) \subset F(\mathrm{id}_{C_0})^{-1}(X(C_0)) = X(C_0)$$

which gives the second inclusion $\supset$.

If X is atomic, then for all C, $\operatorname{card}(X(C)) = 1$, hence, for all $c : C \to C_0$, $\operatorname{card}(F(c)(X(C))) = 1$. Of course $F(c)(X(C)) \subset X(C_0)$ as X is a subfunctor of F, which yields $F(c)(X(C)) = X(C_0)$. □

Lemma 3.3. *If X is a subfunctor of F and $U : \mathrm{Ob}(\mathscr{C}) \to Sets$ is a function such that $X \subset U$, then $X \subset \overline{U}$.*

Proof. If X is a subfunctor of F such that $X \subset U$ then it follows from Lemma 3.2 that, for each object C_0 of $\mathrm{Ob}(\mathscr{C})$:

$$X(C_0) \subset \bigcap_{c:C_0 \to C} F(c)^{-1}(U(C))$$

Thence the result according to $(\star)$ $\square$

Definition 3.4 (Subfunctors complying with a partial choice)**.** A *partial choice* $\mathbb{P}$ *(of F)* is a partial function $\mathrm{Ob}(\mathscr{C}) \to \bigcup_{C \in \mathscr{C}} F(C)$ such that for each C in the domain of $\mathbb{P}$, $\mathbb{P}(C) \in F(C)$. We will often write such a $\mathbb{P}$ as a set of pairs $\{(C, \mathbb{P}(C)), (C', \mathbb{P}(C')), \ldots\}$. We call $\mathbb{P}$ *truly partial* when $\mathrm{dom}(\mathbb{P}) \subsetneq \mathrm{dom}(F)$.

A subfunction and thus, a subfunctor V of F, is said to *comply with a partial choice* $\mathbb{P}$ when for each $C \in \mathrm{dom}(\mathbb{P})$, $V(C) = \{\mathbb{P}(C)\}$.

Given a function $U \subset F$ and a partial choice $\mathbb{P}$, we write $\mathbb{P} \in U$ if $\mathbb{P}(C) \in U(C)$ for all $C \in \mathrm{dom}(\mathbb{P})$ and $\mathbb{P} \notin U$ otherwise.

For convenience, in the description of the algorithm, we write $\mathbb{P}$ as a set of pairs. The use of the notion of partial *function* makes implicit the fact that one and only one element of $F(C)$ is chosen per C to specify $\mathbb{P}$. In the following, an atomic subfunctor of F will also be seen as a "non-truly partial" choice of F by "forgetting" the action of F on arrows, so we can also describe it as a set of pairs $\{(C, \mathbb{P}(C)) \mid C \in \mathscr{C}\}$.

Definition 3.5. Given a function $U \subset F$ and a partial choice $\mathbb{P}$, $\mathrm{Atom}^F(U, \mathbb{P})$ is defined as the set of all atomic subfunctors of $U \subset F$ that comply with $\mathbb{P}$. Readily, $\mathbb{P} \notin U$ implies that $\mathrm{Atom}^F(U, \mathbb{P}) = \varnothing$. Also, note that the set of all atomic subfunctors of F is exactly $\mathrm{Atom}^F(F, \varnothing)$.

Lemma 3.6. *Consider a function $U \subset F$ and a partial choice $\mathbb{P} \in U$. If $\mathbb{P} \notin \overline{U}$ then* $\mathrm{Atom}^F(U, \mathbb{P}) = \varnothing$.

Proof. Suppose that $\mathrm{Atom}^F(U, \mathbb{P}) \neq \varnothing$ and that $X \in \mathrm{Atom}^F(U, \mathbb{P})$. We thus have $X \subset \overline{U}$ by Lemma 3.3 . Therefore, for all $C \in \mathrm{dom}\,\mathbb{P}$, $X(C) = \{\mathbb{P}(C)\} \subset \overline{U}(C)$. Thence the result by contraposition. $\square$

Lemma 3.7. *For any function $U \subset F$ and any partial choice $\mathbb{P}$:*

$$\mathrm{Atom}^F(U, \mathbb{P}) = \mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right)$$

Proof. Consider a function $U \subset F$ and a partial choice $\mathbb{P}$. If $\mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right) \neq \varnothing$ then, for any $X \in \mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right)$, $X \subset \overline{U} \subset U$. Therefore, we have the implication:

$$\mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right) \neq \varnothing \Rightarrow \mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right) \subset \mathrm{Atom}^F(U, \mathbb{P})$$

On the other hand, if $\mathrm{Atom}^F(U, \mathbb{P}) \neq \varnothing$, Lemma 3.6 implies that $\mathbb{P} \in \overline{U}$. If $X \in \mathrm{Atom}^F(U, \mathbb{P})$ then $X \subset \overline{U}$ by Lemma 3.3. Thereby X is atomic, complies with $\mathbb{P} \in \overline{U}$ and $\overline{U} \subset F$ as the maximal subfunctor of F contained in U. This means that $X \in \mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right)$. As a consequence,

$$\mathrm{Atom}^F(U, \mathbb{P}) \neq \varnothing \Rightarrow \mathrm{Atom}^F(U, \mathbb{P}) \subset \mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right)$$

If $\mathrm{Atom}^F(U, \mathbb{P}) = \varnothing$ (resp. $\mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right)) = \varnothing$) the two implications above show that $\mathrm{Atom}^F\left(\overline{U}, \mathbb{P}\right) = \varnothing$ (resp. $\mathrm{Atom}^F(U, \mathbb{P})) = \varnothing$). $\square$

Definition 3.8. Given a function $U \subset F$ and a partial choice $\mathbb{P}$ of F, we define the function $U^{\mathbb{P}}$ by setting, for each $C \in \mathrm{Ob}(\mathscr{C})$:

$$U^{\mathbb{P}}(C) = \begin{cases} \{\mathbb{P}(C)\} & \text{if } C \in \mathrm{dom}\,\mathbb{P}, \\ U(C) & \text{otherwise} \end{cases} \tag{1}$$

Readily, with the same notation as in the definition above, $U^{\mathbb{P}}$ is a subfunction of F. Further, we can state the following lemma, which directly follows from the definition above and whose proof is left to the reader.

Lemma 3.9. *Given a function $U \subset F$ and a partial choice $\mathbb{P}$ of F, we have:*

1. *If a subfunction $X \subset U$ of F complies with $\mathbb{P}$ then $X \subset U^{\mathbb{P}}$*
2. *If $\mathbb{P} \in U$ then $U^{\mathbb{P}}$ is a subfunction of U*

Lemma 3.10. *Given a function $U \subset F$ and a partial choice $\mathbb{P}$, we have*

$$\mathrm{Atom}^F(U,\mathbb{P}) = \mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right)$$

Proof. Suppose that $\mathrm{Atom}^F(U,\mathbb{P}) \neq \varnothing$. If $X \in \mathrm{Atom}^F(U,\mathbb{P})$, then $X \subset U$ and X complies with $\mathbb{P}$. Thus, by item 1 of Lemma 3.9, $X \subset U^{\mathbb{P}}$. Therefore, if $\mathrm{Atom}^F(U,\mathbb{P}) \neq \varnothing$ then $\mathrm{Atom}^F(U,\mathbb{P}) \subset \mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right)$, which in turn implies that $\mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right) \neq \varnothing$.

Conversely, suppose that $\mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right) \neq \varnothing$. If $X \in \mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right)$, then X complies with $\mathbb{P}$. In addition, given any $C \in \mathscr{C}$, $X(C) \subset U^{\mathbb{P}}(C)$. If $C \in \mathrm{dom}\,\mathbb{P}$, $U^{\mathbb{P}}(C) = \{\mathbb{P}(C)\}$. Since $\mathbb{P} \subset U$, $\{\mathbb{P}(C)\} \subset U(C)$ and thus $X(C) \subset U(C)$. On the other hand, if $C \notin \mathrm{dom}\,\mathbb{P}$, $U^{\mathbb{P}}(C) = U(C)$ and we thereby have $X(C) \subset U(C)$ again. Because X is an atomic subfunctor of F, we derive from the foregoing that $\mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right) \subset \mathrm{Atom}^F(U,\mathbb{P})$, which concludes the proof. □

As a direct corollary of Lemmas 3.7 and 3.10, we have:

Proposition 3.11. *Given a function $U \subset F$ and a partial choice $\mathbb{P}$ of F,*

$$\mathrm{Atom}^F(U,\mathbb{P}) = \mathrm{Atom}^F\left(\overline{U},\mathbb{P}\right) = \mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right) = \mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}},\mathbb{P}\right)$$

Corollary 3.12. *Given a function $U \subset F$ and a partial choice $\mathbb{P}$, if there exists an object C of $\mathscr{C}$ such that $\overline{U^{\mathbb{P}}}(C) = \varnothing$ then* $\mathrm{Atom}^F(U,\mathbb{P}) = \varnothing$.

Proof. If $\overline{U^{\mathbb{P}}}(C) = \varnothing$ for some object C of $\mathscr{C}$, then it follows from Lemma 3.3 that $\mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right) = \varnothing$. Whence the result by Proposition 3.11. □

Proposition 3.13. *Given a function $U \subset F$ and a partical choice $\mathbb{P}$,*

$$\forall C \in \mathrm{Ob}(\mathscr{C}), \mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) = 1 \Rightarrow \mathrm{Atom}^F(U,\mathbb{P}) = \left\{\overline{U^{\mathbb{P}}}\right\}$$

Proof. Suppose that $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) = 1$ for all $C \in \mathrm{Ob}(\mathscr{C})$. Since $\overline{U^{\mathbb{P}}} \subset U^{\mathbb{P}}$, $\overline{U^{\mathbb{P}}}$ is an atomic subfunctor of $U^{\mathbb{P}} \subset F$. In addition, if $C \in \mathrm{dom}\,\mathbb{P}$, $\overline{U^{\mathbb{P}}}(C) \subset U^{\mathbb{P}}(C) = \{\mathbb{P}(C)\}$, which implies that $\overline{U^{\mathbb{P}}}(C) = \{\mathbb{P}(C)\}$ by the assumed atomicity of $\overline{U^{\mathbb{P}}}$. Thereby, $\overline{U^{\mathbb{P}}}$ complies with $\mathbb{P}$ and is thus an element of $\mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right)$. It follows from Proposition 3.11 that $\overline{U^{\mathbb{P}}} \in \mathrm{Atom}^F(U,\mathbb{P})$.

Now, let X be any element of $\mathrm{Atom}^F(U,\mathbb{P})$. According to Corollary 3.11, $X \in \mathrm{Atom}^F\left(U^{\mathbb{P}},\mathbb{P}\right)$. Therefore, by Lemma 3.3 , $X \subset \overline{U^{\mathbb{P}}}$. Since X and $\overline{U^{\mathbb{P}}}$ are atomic, this inclusion implies that $X = \overline{U^{\mathbb{P}}}$. □

Definition 3.14. Given two partial choices $\mathbb{P}$ and $\mathbb{P}'$ of F, we say that $\mathbb{P} \prec \mathbb{P}'$ if $\mathrm{dom}\,\mathbb{P} \subset \mathrm{dom}\,\mathbb{P}'$ and for any $C \in \mathrm{dom}\,\mathbb{P}$, $\mathbb{P}(C) = \mathbb{P}'(C)$.

Lemma 3.15. *Given a function $U \subset F$ and two partial choices $\mathbb{P} \subset U$ and $\mathbb{P}' \subset U$ of F, if $\mathbb{P} \prec \mathbb{P}'$ then* $\mathrm{Atom}^F(U,\mathbb{P}') \subset \mathrm{Atom}^F(U,\mathbb{P})$

Proof. If X is an atomic sunfunctor of $U \subset F$ that complies with a partial $\mathbb{P}' \in U$ of F then, for any object C belonging to $\mathrm{dom}\,\mathbb{P}'$, $X(C) = \{\mathbb{P}'(C)\}$. If, in addition, $\mathbb{P} \subset U$ is another partial choice of F such that $\mathbb{P} \prec \mathbb{P}'$ then, given any element C of $\mathrm{dom}\,\mathbb{P}$, $\mathbb{P}(C) = \mathbb{P}'(C)$ and the result follows. □

Proposition 3.16. *Consider a function $U \subset F$ and a partial choice $\mathbb{P}$ of F. Set*

$$\mathscr{S} = \left\{ C \in \mathrm{Ob}(\mathscr{C}) \mid \mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) > 1 \right\}$$

If $\mathscr{S} \neq \varnothing$ then, $\forall C \in \mathscr{S}$,

$$\mathrm{Atom}^F(U,\mathbb{P}) = \bigcup_{E \in \overline{U^{\mathbb{P}}}(C)} \mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C,E)\}\right)$$

Proof. Suppose that $\mathscr{S} \neq \varnothing$and consider any $C \in \mathscr{S}$. Let E be any element of $\overline{U^{\mathbb{P}}}(C)$. Since $\mathbb{P} \subset \mathbb{P} \cup \{(C,E)\}$, it follows from Lemma 3.15 that $\mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C,E)\}\right) \subset \mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P}\right)$ and we derive from Proposition 3.11 that $\mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C,E)\}\right) \subset \mathrm{Atom}^F(U,\mathbb{P})$. Therefore, for any $C \in \mathscr{S}$,

$$\bigcup_{E \in \overline{U^{\mathbb{P}}}(C)} \mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C,E)\}\right) \subset \mathrm{Atom}^F(U,\mathbb{P})$$

Conversely, if $\mathrm{Atom}^F(U,\mathbb{P}) = \varnothing$, the inclusion above induces directly the inequality. Thus, suppose that $\mathrm{Atom}^F(U,\mathbb{P}) \notin \varnothing$ and pick any $X \in \mathrm{Atom}^F(U,\mathbb{P})$ and any $C \in \mathscr{S}$. Since X is atomic, there exists a set E such that $X(C) = \{E\}$. In addition, we have $X(C) \subset U^{\mathbb{P}}(C)$ because $X \in \mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P}\right)$ by Proposition 3.11. Therefore, $E \in \overline{U^{\mathbb{P}}}$. Since X complies with $\mathbb{P}$, it also complies with $\mathbb{P} \cup \{(C,E)\}$. We thus conclude that $X \in \mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C,E)\}\right)$, which concludes the proof. □

We have now all the material to prove our main Theorem 3.17 below, which establishes the convergence to $\mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P}\right)$ of Procedure EnumerateAtomic.

Theorem 3.17. *Suppose that $\mathscr{C}$ is a category such that $\mathrm{Ob}(\mathscr{C})$ is a finite set and consider any functor $F : \mathscr{C} \to Sets$. Let $\mathscr{U}$ be the set of all subfunctions $U \subset F$ and $\mathscr{P}$ be the set of all partial choices $\mathbb{P}$ of F.*

The function $\mathrm{Atom}^F(-,-) : \mathscr{U} \times \mathscr{P} \to \mathrm{Ob}(Sets)$ that assigns $\mathrm{Atom}^F(U,\mathbb{P})$ to any given $(U,\mathbb{P}) \in \mathscr{U} \times \mathscr{P}$ is the unique function $\mathrm{EA}^F(-,-) : \mathscr{U} \times \mathscr{P} \to \mathrm{Ob}(Sets)$ such that:

(P_1) *For any $(U,\mathbb{P}) \in \mathscr{U} \times \mathscr{P}$ for which exists $C \in \mathrm{Ob}(\mathscr{C})$ such that $\overline{U^{\mathbb{P}}}(C) = \varnothing$,*

$$\mathrm{EA}^F(U,\mathbb{P}) = \varnothing$$

(P_2) *For any $(U,\mathbb{P}) \in \mathscr{U} \times \mathscr{P}$ such that, for all $C \in \mathrm{Ob}(\mathscr{C})$, $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) = 1$,*

$$\mathrm{EA}^F(U,\mathbb{P}) = \left\{\overline{U^{\mathbb{P}}}\right\}$$

(P_3) *For any $(U,\mathbb{P}) \in \mathscr{U} \times \mathscr{P}$ such that $\mathscr{S} = \left\{ C \in \mathrm{Ob}(\mathscr{C}) \mid \mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) > 1 \right\} \neq \varnothing$,*

$$\forall C \in \mathscr{S}, \mathrm{EA}^F(U,\mathbb{P}) = \bigcup_{E \in \overline{U^{\mathbb{P}}}(C)} \mathrm{EA}^F(\overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C,E)\})$$

Proof. First, note that (P_1), (P_2) and (P_3) are exclusive and exhaustive of all possible cases and according to Corollary 3.12, Proposition 3.13 and Proposition 3.16, $\mathrm{Atom}^F(-,-)$ satisfies these three properties.

Conversely, suppose that $\mathrm{EA}^F(-,-) : \mathscr{U} \times \mathscr{P} \to \mathrm{Ob}(Sets)$ satisfies (P_1), (P_2) and (P_3). Set $N = \mathrm{card}(\mathrm{Ob}(\mathscr{C}))$ and for any $n \in [\![0,N]\!]$, define:

$$\mathscr{P}_n = \{\mathbb{P} \in \mathscr{P} \mid \mathrm{card}(\mathrm{Ob}(\mathscr{C}) \setminus \mathrm{dom}\,\mathbb{P}) = n\}$$

We then establish by recursion that, for any given $n \in [\![0,N]\!]$, any pair $(U,\mathbb{P}) \in \mathscr{U} \times \mathscr{P}_n$, $\mathrm{Atom}^F(U,\mathbb{P}) = \mathrm{EA}^F(U,\mathbb{P})$.

First, consider the case $n = 0$.

We have $\mathscr{P}_0 = \{\mathbb{P} \in \mathscr{P} \mid \operatorname{dom}\mathbb{P} = \mathrm{Ob}(\mathscr{C})\}$. Therefore, for any $(U,\mathbb{P}) \in \mathscr{U} \times \mathscr{P}_0$ and any $C \in \mathrm{Ob}(\mathscr{C})$, $U^{\mathbb{P}}(C) = \{\mathbb{P}(C)\}$ and since $\overline{U^{\mathbb{P}}}(C) \subset U^{\mathbb{P}}(C)$, $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) \leqslant 1$.

We thus have two subcases only. If there exists $C \in \mathrm{Ob}(\mathscr{C})$ such that $\overline{U^{\mathbb{P}}}(C) = \varnothing$, it follows from (P_1) and Corollary 3.12 that $\mathrm{EA}^F(U,\mathbb{P}) = \mathrm{Atom}^F(U,\mathbb{P}) = \varnothing$. Otherwise, for all $C \in \mathrm{Ob}(\mathscr{C})$, $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) = 1$. We thus derive from (P_2) and Proposition 3.13 that $\mathrm{EA}^F(U,\mathbb{P}) = \mathrm{Atom}^F(U,\mathbb{P}) = \left\{\overline{U^{\mathbb{P}}}\right\}$. Thence the result holds true for $n = 0$.

Suppose now that the result is true for a given $n \in [\![0,N-1]\!]$. Let $(U,\mathbb{P}) \in \mathscr{U} \times \mathscr{P}_{n+1}$. If there exists $C \in \mathrm{Ob}(\mathscr{C})$ such that $\overline{U^{\mathbb{P}}}(C) = \varnothing$, it follows from (P_1) and Corollary 3.12 that $\mathrm{EA}^F(U,\mathbb{P}) = \mathrm{Atom}^F(U,\mathbb{P})$. Otherwise, if $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) \neq \varnothing$ for all $C \in \mathrm{Ob}(\mathscr{C})$, we have the following two subcases. On the one hand, if $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) = 1$ for all $C \in \mathrm{Ob}(\mathscr{C})$, $(P_{2,n+1})$ and Proposition 3.13 imply that $\mathrm{EA}^F(U,\mathbb{P}) = \mathrm{Atom}^F(U,\mathbb{P}) = \left\{\overline{U^{\mathbb{P}}}\right\}$. On the other hand, if there exists $C \in \mathrm{Ob}(\mathscr{C})$ such that $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) > 1$, C is no element of $\operatorname{dom}\mathbb{P}$ because, otherwise, $U^{\mathbb{P}}(C)$ would be $\{\mathbb{P}(C)\}$ and we would have $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) \leqslant 1$, a contradiction. Therefore, given any $E \in \overline{U^{\mathbb{P}}}(C)$, $\mathbb{P} \cup \{(C,E)\} \in \mathscr{P}_n$. Since we assume that the result is true for n, it follows from Proposition 3.11 that $\mathrm{EA}^F(\overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C,E)\}) = \mathrm{Atom}^F\left(\overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C,E)\}\right)$ for any $E \in \overline{U^{\mathbb{P}}}(C)$. This, according to (P_3), $\mathrm{EA}^F(U,\mathbb{P}) = \mathrm{Atom}^F(U,\mathbb{P})$. $\square$

Procedure EnumerateAtomic straightforwardly follows from Theorem 3.17.

By a rapid analysis of the algorithm, and assuming that $\mathscr{C}$ is a finite category and each $F(C)$ is a finite set, we derive that its worst case time complexity is:

$$O\left(|\mathrm{Ob}(\mathscr{C})| + |\mathrm{Mor}(\mathscr{C})| + \left(\max_{C \in \mathscr{C}}(|F(C)|)\right)^{|\mathrm{Ob}(\mathscr{C})| - |\operatorname{dom}\mathbb{P}|}\right)$$

4 Using the enumeration

As mentioned in the introduction, the algorithm EnumerateAtomic is useful in the context of clusters [6], as clusters are a special case of atomic subfunctors.

Consider the functor $\pi_0 : Cat \to Sets$ of connected components so that $\pi_0(\mathscr{C})$ is the set of connected components of $\mathscr{C}$. Let $\mathscr{C}$ be a small category. Let $P : \mathscr{P} \to \mathscr{C}$ and $Q : \mathscr{Q} \to \mathscr{C}$ be two diagrams to $\mathscr{C}$. We define the functor:

$$\mathrm{CC}_{P,Q} : p \to \pi_0((P(p) \downarrow Q))$$

where $(- \downarrow -)$ denotes the comma-category.

A cluster G is defined as an element of the set $\operatorname*{Lim}_p \operatorname*{Colim}_q \mathrm{Hom}_{\mathscr{C}}(P(p), Q(q))$, or alternatively as an atomic subfunctor of $\mathrm{CC}_{P,Q}$ [5, Proposition 4.4.4, page 121].

Corollary 4.1. $\operatorname*{Lim}_p \operatorname*{Colim}_q \mathrm{Hom}_{\mathscr{C}}(P(p), Q(q)) = \mathrm{Atom}^F(\mathrm{CC}_{P,Q}, \mathrm{CC}_{P,Q}, \varnothing)$

Clusters are a crucial part of the categorical representation of systems [8], because they represent the interactions between subsystems (seen as diagrams). In particular, their presence or absence between two diagrams $D : \mathscr{D} \to \mathscr{C}$ and $D' : \mathscr{D}' \to \mathscr{C}$ matters in the Multiplicity Principle [8, Part A, Chapter 3, Section 4.3, pages 92-94]:

Definition 4.2 (Multiplicity Principle)**.** Let $D : \mathscr{D} \to \mathscr{C}$ and $D' : \mathscr{D}' \to \mathscr{C}$ be two diagrams to $\mathscr{C}$.

We say that D and D' verify the Multiplicity Principle (MP) when:

Input: A functor F, a function $U \subset F$, a set $\mathbb{P}$ of pairs $(C, E \in F(C))$
Output: The set $\mathrm{Atom}^F(U, \mathbb{P})$ of atomic subfunctors X of F contained in U and that comply with $\mathbb{P}$, that is, such that for all $(C,E) \in \mathbb{P}$, $X(C) = \{E\}$

`/* Initialize the procedure by constructing` $U^{\mathbb{P}}$ `*/`

foreach $C \in \mathscr{C}$ **do**
  if *there is a pair* $(C,E) \in \mathbb{P}$ **then**
    Set $U^{\mathbb{P}}(C) = \{E\}$;
  else
    Set $U^{\mathbb{P}}(C) = U(C)$;
  end
end
Compute $\overline{U^{\mathbb{P}}}$;
if *there is a C such that* $\overline{U^{\mathbb{P}}}(C) = \varnothing$ **then**
  `/* There will be no atomic subfunctor, by Theorem 3.17 (see` (P_1)`) or Corollary 3.12. */`
  Return $\varnothing$;
end
if *for all* $C \in \mathscr{C}$, $\overline{U^{\mathbb{P}}}(C) \cong 1$ **then**
  `/* We are in the case covered by` (P_2) `in Theorem 3.17 or Proposition 3.13 stating that` $\overline{U^{\mathbb{P}}}$ `is the unique atomic subfunctor of` F `contained in` U `and complying with` $\mathbb{P}$`. */`
  Return $\{X\}$;
end
if *there is a* $C \in \mathscr{C}$ *such that* $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C)\right) > 1$ **then**
  `/* We thus proceed iteratively as established by` (P_3) `in Theorem 3.17 or Proposition 3.16. */`
  Let $\mathrm{Res} = \varnothing$;
  foreach C_1 *such that* $\mathrm{card}\left(\overline{U^{\mathbb{P}}}(C_1)\right) > 1$ **do**
    foreach $E_1 \in \overline{U^{\mathbb{P}}}(C_1)$ **do**
      $\mathrm{Res} = \mathrm{Res} \cup \mathrm{EnumerateAtomic}\left(F, \overline{U^{\mathbb{P}}}, \mathbb{P} \cup \{(C_1, E_1)\}\right)$
    end
  end
  Return Res
end

Algorithm 1: EnumerateAtomic()

1. $Cocones(D)$ and $Cocones(D')$ are isomorphic
2. $\text{peak}(Cocones(D)) = \text{peak}(Cocones(D'))$ (the cocones to D and D' have the same peaks)
3. For all cluster $G : D \to D'$ or $G : D' \to D$, the composition functor $\Omega G : \delta \mapsto \delta \circ G$ is not an isomorphism.

The MP is our main lead for the representation of emergence [8] and resilience [11] in complex systems. The final goal consists in studying real-world systems through category theory, and thus, a computable way of verifying the MP in a category representing a system has value. The Algorithm DetectMP() provides us with a means to check whether a category satisfies the MP.

Input: Two diagrams $D : \mathscr{D} \to \mathscr{C}$ and $D' : \mathscr{D}' \to \mathscr{C}$
Output: Whether or not D and D' verify the MP
`/* We first collect the cocones of` D `and` D' `*/`
1 $\text{Cocones}_D, \text{Cocones}_{D'} = [\,], [\,]$;
2 **foreach** $C \in \mathscr{C}$ **do**
3 | **foreach** *cocone* $\delta : D \to C$ **do**
4 | | Append δ to Cocones_D ;
5 | **end**
6 | **foreach** *cocone* $\delta' : D \to C$ **do**
7 | | Append δ' to $\text{Cocones}_{D'}$;
8 | **end**
9 **end**
10 **if** Cocones_D *and* $\text{Cocones}_{D'}$ *are not isomorphic* **then**
11 | Return FALSE ;
12 **end**
13 **foreach** *cluster* $G \in \text{EnumerateAtomic}(\text{CC}_{P,Q}, \text{CC}_{P,Q}, \varnothing)$ **do**
14 | Construct the composition functor $\Omega G : \delta' \mapsto \delta' \circ \alpha$;
15 | Compute $\Omega G(\text{Cocones}_{D'})$;
16 | **if** $\text{card}(\Omega G(\text{Cocones}_{D'})) = \text{card}(\text{Cocones}_D)$ *and* ΩG *is injective* **then**
17 | | Return FALSE ;
18 | **end**
19 **end**
20 Return TRUE ;

Algorithm 2: DetectMP()

Unfortunately, Algorithm DetectMP() is untractable, as it relies at line 10 on a problem very similar to the graph isomorphism problem, which is known to be NP. It is unknown whether it is simply P or NP-complete [1]. [2] showed that the graph isomorphism problem could be solved in quasipolynomial time (complexity $O\left(n^{P(\log n)}\right)$ where P is a polynomial). Also note that there exist heuristic algorithms that help solve (most cases of) the problem in polynomial time (for example, the Weisfeiler-Leman algorithm [12, 7]).

5 Conclusion

The first presented algorithm gives an explicit, constructible and even, computable (provided that all considered categories, functions and sets are finite) generalisation of [6, Lemma 3.6, Section 3, page 499] to any functor and its atomic subfunctors.

The question of the construction of clusters in a category is useful because clusters, firstly, are the arrows of the free cocompletion, and secondly, are useful to study the properties of systems described in categorical terms, that is, emergence [8] or resilience [11, 5]. The second algorithm is a first attempt the detection of the MP between two diagrams. Of course, it is currently computationally costly. It needs thorough study to be optimised, which is left for future work.

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