Pattern Matching in discrete Models for Ecosystem Ecology

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Abstract: In this paper we consider discrete qualitative models of ecosystems viewed as collections of interacting living (animals, plants...) and nonliving entities (air, water, soil...), whose conditions of appearance/disappearance are controlled by a set of formal rules (i.e., processes). We present here a rule-based method allowing to compare ecosystems. The method relies on a measure of similarity and on an optimization algorithm. In addition, the proposed method allows to detect patterns (i.e., ecological processes or sets of processes) in ecosystems. We have validated the method by applying it against a set of models and patterns provided by ecologists.

1 INTRODUCTION

Ecosystems are defined by complex processes of highly different nature: e.g. bio-ecological, physico-chemical and socio-economical. The dynamics of such systems is difficult to grasp as it is the result of an intricate interplay between a large number of processes: the functioning of living species (fauna and flora) and the dynamics of soil and climate. In addition, all these entities and processes are influenced and often highly impacted by human activities.

Understanding the functioning of ecosystems is thus crucial for a more sustainable management of them. Indeed, we face today fast and dangerous changes of most ecosystems (due to climate change, to human activities...) that we are compelled to understand so to appropriately react. Unfortunately, in practice, the development and analysis of models of ecosystems remain a challenge and constitutes a critical bottleneck as they are usually treated on a case-by-case basis with few generalizations.

One relevant way of improving our understanding of ecosystems functioning is to provide more formal frameworks. They have proven to be valuable for speeding up and better controlling the decision procedures. Similarly to what happens in biology, ordinary differential equations (ODE) are the dominant modeling methodology for ecosystems (May, 1972, Lotka, 1925). The drawbacks of such models are that: i) they usually need to quantify various parameters (mostly unknown). ii) They are not able to faithfully represent the time scale required for observation of ecological processes which is usually large. iii) On top of this, analytic solutions usually do not exist and models often represent averaged and sometimes unrealistic behaviors of ecosystems. In contrast, while discrete qualitative models are high level abstractions of observed processes, they allow unraveling the tangled causal relationships between system's entities (i.e. material constitutive components). The success of discrete qualitative approaches is witnessed, for instance, in systems biology with formalisms like Petri nets (Baldan et al., 2010), Boolean networks (Thomas, 1973), process algebras (Cardelli, 2005) and rewriting systems (Giavitto et al., 2004), to cite a few.

In ecology, discrete qualitative modelling is still pioneering and under exploited. Approaches such as (Gaucherel et al., 2012, Gaucherel et al., 2014), where the authors study the driving rules needed to change agricultural mosaics and model contrasted landscapes, are promising. However, much more may be obtained by developing original solutions based on the suitable application of existing theory and associated (automated) tools. One of the goals of this paper is to contribute in this regard.

As a starting point of our developments we take a general discrete qualitative formalism proposed in (Gaucherel and Pommereau, 2017). Ecosystems are modeled as a set of (living and nonliving) entities

together with a set of rewriting rules expressing the conditions of their appearance/disappearance (i.e., the ecosystem component responses). These rules may be interpreted as the functioning bricks of landscape modelling. Each rule is, thus, part of a broader process describing the behavior of the whole ecosystem.

Yet, there are processes that are common to several ecosystems: e.g.–for species interactions– predation, competition, symbiosis... and it is crucial to be able to identify them to better describe the ecosystem under study. Hence, we can raise the following questions: How can we detect whether a given process is present in an ecosystem? Is the introduction of a new entity causing the appearance of a known process? Indeed, to detect wanted or unwanted interaction patterns would guide decisions for taking actions according to the management objectives, such as preventing or reinforcing some ecosystemic processes or states. Identify certain ecological processes or *interaction patterns* –in a more computer science oriented terminology– by employing classical graph-theoretical methods on the state space is ineffective. Indeed, in realistic ecosystem models, the modeled dynamics usually leads to huge state spaces (often hundreds of thousands of states). It is more efficient to search for patterns by referring only to the (limited) syntactical system specification as similar processes look similar at the rule level.

From a more general point of view, a pattern search corresponds to a variant of the problem of assessing the similarity between models of ecosystems. In order to compare two models of ecosystems, we introduce a pair of mappings, the first identifying entities and the latter rules, and a similarity measure expressed as a scoring function. This scoring majors the number of matched entities and rules, and penalizes those that do not perfectly match. Similarity is then defined as an optimization problem through the scoring function. Indeed, the scoring function with optimal value uniquely determines the mappings of entities and rules. This way the definition of the scoring function is used to search for interaction patterns in the rule-based models of ecosystems. As the complexity of this kind of search is exponential, it is not always possible in realistic cases to find optimal solutions in a reasonable time. Nevertheless, optimization tools generally allow obtaining a sub-optimal solution quite efficiently, solutions that can then be refined.

We implemented a prototype that allows encoding the matching of two models into a pseudo-Boolean optimization problem and invoking tool Sat4j (Le Berre and Parrain, 2010) to solve it. We applied this prototype to systematically match a collection of predefined interaction patterns against a set of models of "real" ecosystems.

The paper is structured as follows: Section 3 introduces the formal modeling of ecosystems we have used and presents running examples. Section 4 defines similarity measures used to compare ecosystems and discusses possible extensions of them. Several comparisons between ecosystems are used as illustrations for the scoring function. In Section 5, we present the results of our main case study: a search of interaction patterns in realistic ecosystems. Next section 2 is devoted to an overview of related work, while some concluding remarks and perspectives are presented in Section 6.

2 Related work

The model of ecosystems developed in this paper is an instance of the more general family of rewriting systems (Terese, 2003). Such systems have been shown convenient in formalizing models, in particular for systems biology and chemistry. In these domains, we thus find formalizations that are reminiscent of ours: the Biocham (Fages and Soliman, 2008), the κ-calculus (Danos and Laneve, 2004), reaction systems (Ehrenfeucht and Rozenberg, 2007), activity networks (Delaplace et al., 2018), P-systems (Paun et al., 2011), cellular automata (Gaucherel, 2006, Agnihotri and Sharma, 2015) that describe the evolution of cells and/or molecules applying rewriting rules.

Yet, the question of similarity appears rather novel in rewriting systems. In a broader context, it is usually associated to the notion of equivalence. In concurrent systems like ours, equivalences are usually semantics based, notable examples are partial ordering equivalences, trace equivalence (van Glabbeek and Goltz, 1989), bisimulation (Sangiorgi, 2011), principal transition sequences (Wang et al., 2010), etc. These notions are usually explored in theory and tailored to highly abstracted languages, moreover computed with a few existing tools. In practice, we cannot expect to use such approaches on the huge state spaces generated from detailed and realistic (qualitative) models of ecosystems.

Works that are closer to ours can therefore be found in domains in which models use structural aspects rather than their behaviors. For instance in systems biology, several similarity measures can be found (a good survey summarizing the used techniques may be found in (Henkel et al., 2018)). Technically speaking, these methods include the analysis of similar pathways through a structural approach, namely the search of t-invariants in Petri net models (Baldan et al., 2013a, Baldan et al., 2013b,

Grafahrend-Belau et al., 2008). They also define a similarity score, but our goal and underlying modelling are considerably different.

Another domain that focuses on similarity rates is business process modeling. For instance in (Xiao et al., 2009), the authors evaluate the similarity of Petri nets by comparing the set of structural elements such as places and transition arcs. Similarity is based on rates of identical elements. Instead, our approach is finer-grained and more flexible: the mappings allow different names of entities and rules, and we allow partially matched rules. In (Bae et al., 2006), process-based models are studied and similarity is defined on sets of nodes as the proportion of matched ones. Yet, these authors do not deal with relations between them. Likewise, in (Dijkman et al., 2011), other similarities are explored. In this context the authors still compare structural elements of workflows (e.g. sets of nodes), but they allow different kinds of distance measures: string-edit distance, labels synonyms and contextual similarity. The latter measure is the closest to ours, as we consider separately the input (or conditions, the left hand side of a rule) and the output (realization, the right hand side of a rule) of a node. Conversely, here, we take into consideration penalties for elements that are not matched. The work in (Dijkman et al., 2011) shows how similarities in business process model are linked to the semantic web domain, a survey of which on corresponding metrics can be found in (Euzenat and Shvaiko, 2007).

Finally, concerning explicitly the pattern search, the work in (Milo et al., 2002) has analogous goals. These authors search for patterns by counting the number of occurrences of a given subgraph in specific networks (world wide web, electronic circuits, ...) and comparing it to the number of occurrences in random generated networks. This approach is completely different to ours, as their method applies to graphs while ours applies to "hyper-graphs". Moreover, they use techniques from statistics while we do not.

3 MODELED ECOSYSTEMS

In this section, we recall the formal definition of a model of an ecosystem as given in (Gaucherel and Pommereau, 2017). An ecosystem consists of a set of *entities* E that can be present (On) or absent (Off). We assume that no entity may be simultaneously On and Off. The status (the presence) of an entity a is called polarity, we use $a+$ to denote that a is On, $a-$ to denote that a is Off. The set of entities E with polarities $\mathsf{p} \in \{+,-\}$ is $\mathsf{E}^{\mathsf{p}} = \{a+, a- \mid a \in \mathsf{E}\}$. The presence of those entities is regulated by a sets of rewriting *rules* R. More formally:

Definition 1 (Ecosystem)**.** *An* ecosystem $\mathcal{E}$ *is a tuple* (E,R) *such that:*

- E *is a set of entities,*
- R *is a set of rewriting rules of the form* $r : \alpha^+, \alpha^- \gg \omega^+, \omega^-$, *where r is the name of the rule,* α^+ *and* ω^+ *are sets of entities that are* On*, and* α^- *and* ω^- *are sets of entities that are* Off.

We denote by $\mathsf{lhs}(r)$ (respectively $\mathsf{rhs}(r)$) the set of entities in the left (respectively right) hand side of the rule r.

An ecosystem state s is defined by the information about the presence or absence of all its entities. It is described as the set of entities that are currently On: thus $s \subseteq \mathsf{E}$, and we assume that the remaining entities $\mathsf{E} \setminus s$ are Off.

The dynamics of an ecosystem (E,R) is parametric over its initial state s_0. It comprises all reachable states obtained by asynchronously applying the rules in R, in a non-deterministic way. A rule r is enabled at a state s if the rule's left hand side, i.e., (α^+,α^-), matches the entities defining s. It means that $\alpha^+ \subseteq s$ and $\alpha^- \cap s = \emptyset$. If it is the case, the rule may apply and a new state s' is generated by updating s according to the rule's right hand side: $s' = (s \setminus \omega^-) \cup \omega^+$.

Example 1 (Pond)**.** *We consider a toy-model of a pond populated with two species of fish, piscivorous and insectivorous ones. The pond behavior is described by the following rules:*

1. if the pond disappears, all fish species disappear too,
2. in summer the pond dries and disappears,
3. if the pond is not dried, both species of fish may live in it,
4. if the piscivorous fish are present, insectivorous fish disappear,
5. if insectivorous fish disappear, piscivorous fish disappear too.

It consists of four entities: the summer, the pond, and two kinds of fish (piscivorous and insectivorous); and seven rules (see Table 1): Rules 1–5 correspond to items 1–5 above, and rules 6 and 7 are used to simulate the change of the seasons.

As an example of the dynamics, let $s_0 = \{P\}$ *be the initial state. Then rule 3 is enabled and its application gives* $s' = \{P,IF,PF\}$*. The whole dynamics is then a directed graph whose vertices are the reachable states and whose edges correspond to the application of rules.* ◇

entities:

Su:	Summer
P:	Pond
PF:	Piscivorous Fish
IF:	Insectivorous Fish

rules:

1: P−	$\gg$ PF−, IF−
2: Su+	$\gg$ P−
3: P+	$\gg$ PF+, IF+
4: PF+	$\gg$ IF−
5: IF−	$\gg$ PF−
6: Su+	$\gg$ Su−
7: Su−	$\gg$ Su+

Table 1: Entities and Rules for Example 1

entities:

B:	Birds
I:	Insects
Pe:	Pesticide
R:	Rain

rules :

1': B+	$\gg$ I−
2': I−	$\gg$ B−
3': Pe−, R+	$\gg$ I+
4': Pe+	$\gg$ I−
5': R+	$\gg$ Pe−
6': B−, Pe−	$\gg$ I+

Table 2: Entities and Rules for Example 2

Example 2 (Pesticides)**.** *As a second small example, consider a fragment of another ecosystem with four entities: birds, insects, pesticides and rain.*

The ecosystem is governed by the following principles: birds eat insects and if insects disappear, birds will vanish as well. As a disturbing factor we add pesticides that may kill insects. Pesticides are washed away by the rain and when there are no pesticides and it is still raining, insects proliferate. Similarly insect proliferation happens when there are no pesticides and no birds. We do not take into account in this example, all the rules (and possibly entities) that are necessary to regulate the presence/absence of rain. Entities and rules are given in Table 2. ◇

4 SIMILARITY BETWEEN ECOSYSTEMS

As mentioned in the introduction, our objective is to identify interaction patterns. An interaction pattern can be considered as a "tiny" ecosystem restricted to few entities and rules. Thus it may be formalized in the same syntax as the one for the whole ecosystem.

entities:

Pred:	Predator
Prey:	Prey

rules:

$1''$: Pred+	$\gg$ Prey−
$2''$: Prey−	$\gg$ Pred−

Table 3: Interaction pattern for predation pattern.

For example, the "habitat" interaction pattern is composed of one entity featuring a specific environment (aquatic, terrestrial, pond, ...) and several entities inhabiting this environment:

1. *if the environment disappears, all inhabitants disappear as well.*

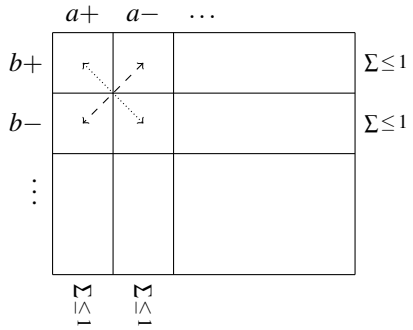
Similarly, an interaction pattern for the "predation" process is composed of two entities and two rules only:

1. *if predators are present, then prey disappear,*
2. *if prey disappear, then predators disappear too.*

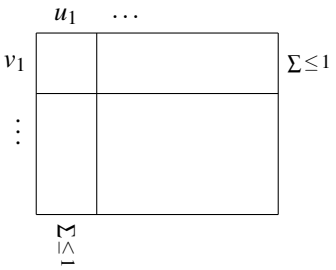
In the example of the pond ecosystem, instances of both above patterns are present. The predation instance is composed of piscivorous and insectivorous species, and of rules 4 and 5; while the habitat instance is composed of entities pond, piscivorous and insectivorous species and of rule 1. Table 3 shows a formal representation of the predation pattern. We may observe that there is a syntactical "similarity" between rules 4 and 5 in the pond ecosystems and rules 1 and 2 in the predation pattern.

The concept of similarity will be the basis of our investigation. Similarity is discussed in theory (see for instance the philosophical work in (Tversky, 1977)) and also used in practice: in law (Mooiman, 2015), in natural sciences (Henkel et al., 2018) and in various branches of computer science. Intuitively, we express it in terms of how many groups of components with the same roles are present in both ecosystems. This means that, given two mappings, between entities and rules respectively, the similarity rate is defined as the number of mapped entities plus how many mapped entities the rules have in common. More formally, let $\mathcal{E}_1 = (\mathsf{E}_1, \mathsf{R}_1)$ and $\mathcal{E}_2 = (\mathsf{E}_2, \mathsf{R}_2)$ be two ecosystems, and μ and ρ be two mappings between entities and rules respectively. The first one is $\mu : \mathsf{E}_1^p \to \mathsf{E}_2^p$. The mapping μ is injective but not necessarily total and polarities are consistent: i.e., if $a+$ is matched with $b-$ then $b+$ is matched with $a-$. It is encoded as a rectangular matrix X of size $(|\mathsf{E}_1^p| \times |\mathsf{E}_2^p|)$ of Boolean values defined for each pair of entities with polarities $(m,n) \in \mathsf{E}_1^p \times \mathsf{E}_2^p$ as

$$X_{m,n} = 1 \text{ if } \mu(m) = n, 0 \text{ otherwise.}$$



(a) The encoding into matrix X of the mapping μ for entities and the illustration of corresponding restrictions.



(b) The encoding of matrix Y of the mapping ρ for the rules and the corresponding restrictions.

Figure 1: Encoding of mappings μ and ρ

In order to implement injectivity and the correspondence between polarities we introduce three restrictions (see Figure 1a):

1. There is at most one "1" in each line:
$$\forall m \in \mathsf{E^p}_1 : \quad \sum_{n \in \mathsf{E^p}_2} X_{m,n} \leq 1;$$
2. There is at most one "1" in each column:
$$\forall n \in \mathsf{E^p}_2 : \quad \sum_{m \in \mathsf{E^p}_1} X_{m,n} \leq 1;$$
3. Polarities are consistently matched:
$$\forall a \in \mathsf{E}_1, b \in \mathsf{E}_2 : \\ X_{a+,b-} = X_{a-,b+} \wedge X_{a+,b+} = X_{a-,b-}.$$

Likewise, the mapping $\rho : \mathsf{R}_1 \to \mathsf{R}_2$ maps the rules. Similarly as for entities, it is encoded as a rectangular matrix Y of size $(|\mathsf{R}_1| \times |\mathsf{R}_2|)$ of Boolean values defined for each pair of rules $(u,v) \in \mathsf{R}_1 \times \mathsf{R}_2$ as

$$Y_{u,v} = 1 \text{ if } \rho(u) = v, 0 \text{ otherwise.}$$

It is subjected to the following restrictions that implements injectivity (see Figure 1b):

1. There is at most one "1" in each line:
$$\forall u \in \mathsf{R}_1 : \quad \sum_{v \in \mathsf{R}_2} Y_{u,v} \leq 1;$$
2. There is at most one "1" in each column:
$$\forall v \in \mathsf{R}_2 : \quad \sum_{u \in \mathsf{R}_1} Y_{u,v} \leq 1.$$

For each pair of mappings (μ,ρ) between ecosystems $\mathcal{E}_1$ and $\mathcal{E}_2$ we define a *scoring* function S. The function assesses the quality of the matching rules with respect to the number of matching entities. The simplest way to express the score is to count, for each pair of matching rules $\rho(u) = v$ (i.e., $Y_{u,v} = 1$), the number of matching entities through function μ on both the left and right hand side (i.e., for each pair of entities n and m in rules u and v respectively, we count the sum of all $X_{n,m} = 1$). The scoring function is a ratio between previous sum and a constant that counts the number of rules times the maximal number of entities in a rule. More precisely:

$$S_0(X,Y) = \frac{1}{\mathbf{T} \cdot \mathbf{r}} \sum_{\substack{u \in \mathsf{R}_1, \\ v \in \mathsf{R}_2}} \left(Y_{u,v} \cdot \sum_{n \in u, m \in v} X_{n,m} \right)$$

where $\mathbf{r} = \min(|\mathsf{R}_1|, |\mathsf{R}_2|)$ is the cardinality of the set of rules in the ecosystem having the smallest number of them, and $\mathbf{T} = \max_{u \in \mathsf{R}_1 \cup \mathsf{R}_2}(|\mathsf{lhs}(u)| + |\mathsf{rhs}(u)|)$ is the maximal number of entities in a rule in both ecosystems, considering at the same time the left ($\mathsf{lhs}(\cdot)$) and right ($\mathsf{rhs}(\cdot)$) hand side. However this simple scoring does not take into account:

1. the different contribution of the left and right hand side. This means, for instance, that a good matching on the left hand side can compensate a bad matching on the right hand one;
2. the proportion of entities that are not matched. Scoring function S_0 does not differentiate between two rule mappings that for a rule in one ecosystem match the same number of entities but the size of matched rules in the second system is different.

Example 3. *For example, take the ecosystems* R_1 *with one rule* $r_1 : A+, B+ \gg C+$ *and* R_2 *with two rules* $r_2 : A+, B+ \gg C+$ *and* $r_3 : A+, B+, D- \gg C+$ *. The score for* ρ_1 *mapping* r_1 *to* r_2 *should be greater than* ρ_2 *mapping* r_1 *to* r_3 *as in the latter the mapping is less perfect and there are entities that are not matched.* $\diamond$

We thus propose a better formulation for the scoring function that takes into account these remarks.

The scoring function is now the sum of the scores of the left hand side and the right hand side and can be summarized as follows:

$$S(X,Y) \stackrel{\text{df}}{=} \frac{1}{\mathbf{r}\cdot(\mathbf{L}+\mathbf{R})} \cdot \sum_{u\in \mathsf{R}_1, v\in \mathsf{R}_2} Y_{u,v}(\mathit{left}(u,v)+\mathit{right}(u,v))$$

where $\mathbf{r} = \min(|\mathsf{R}_1|,|\mathsf{R}_2|)$ as above, $\mathbf{L} = \max_{u\in \mathsf{R}_1\cup \mathsf{R}_2}(|\mathsf{lhs}(u)|)$ and $\mathbf{R} = \max_{u\in \mathsf{R}_1\cup \mathsf{R}_2}(|\mathsf{rhs}(u)|)$ are the maximal numbers of entities occurring in the left (respectively right) hand side of the rules from both ecosystems, and $\mathit{left}(u,v)$ and $\mathit{right}(u,v)$ are the scores for each pair of matching rules $u \in \mathsf{R}_1$ and $v \in \mathsf{R}_2$:

$$\begin{aligned}
\mathit{left}(u,v) = & \sum_{\substack{n\in \mathsf{lhs}(u),\\ m\in \mathsf{lhs}(v)}} X_{n,m} \\
& - \left(\min(|\mathsf{lhs}(u)|,|\mathsf{lhs}(v)|) - \sum_{\substack{n\in \mathsf{lhs}(u),\\ m\in \mathsf{lhs}(v)}} X_{n,m} \right) \\
& - \mathrm{abs}(|\mathsf{lhs}(u)| - |\mathsf{lhs}(v)|) \\
= & \; 2\cdot \sum_{\substack{n\in \mathsf{lhs}(u),\\ m\in \mathsf{lhs}(v)}} X_{n,m} - \min(|\mathsf{lhs}(u)|,|\mathsf{lhs}(v)|) \\
& - \mathrm{abs}(|\mathsf{lhs}(u)| - |\mathsf{lhs}(v)|) \\
\mathit{right}(u,v) = & \; 2\cdot \sum_{\substack{n\in \mathsf{rhs}(u),\\ m\in \mathsf{rhs}(v)}} X_{n,m} - \min(|\mathsf{rhs}(u)|,|\mathsf{rhs}(v)|) \\
& - \mathrm{abs}(|\mathsf{rhs}(u)| - |\mathsf{rhs}(v)|)
\end{aligned}$$

The construction of this scoring function is depicted in Figure 2 below. The part $\mathit{left}(u,v)$ takes the number of matching entities

$$M_L = \sum_{n\in \mathsf{lhs}(u), m\in \mathsf{lhs}(v)} X_{n,m}$$

and subtracts two penalties. The first one: $\min(|\mathsf{lhs}(u)|,|\mathsf{lhs}(v)|) - M_L$ corresponds to the maximum number of entities, which could be matched minus those that are actually matched. The second one: $\mathrm{abs}(|\mathsf{lhs}(u)| - |\mathsf{lhs}(v)|)$ expresses the number of entities which could never be matched because of the difference in the length of the left hand sides of the two rules. This score is maximal when $\mathit{left}(u,v) = \min(|\mathsf{lhs}(u)|,|\mathsf{lhs}(v)|)$ and $|\mathsf{lhs}(u)| = |\mathsf{lhs}(v)|$, i.e., the left hand sides of u and v have the same length, and all their entities match. The part for the right hand sides is defined analogously. The overall score is normalized with respect to the number of rules $\mathbf{r}$ times $\mathbf{L}$ plus $\mathbf{R}$. As an effect of penalties, the score can be negative but it is always between -1 and 1.

Similarity is then defined with respect to the scoring function, as the maximal value it can have with respect to all the possible mappings μ and ρ. It is possible to enumerate all solutions having a score greater than a given threshold.

Also, depending on the specific objective, coefficients may be introduced in the scoring function to weight preferences: the matching of entities and rules can be guided adding additional restrictions or regulating the importance of penalties for not matching parts of the rules.

Example 4 (Similarity)**.** *Let us consider the following pairs of mappings between the ecosystems from Examples 1 and 2:*

1. $\mu_1 = \begin{cases} PF+ \to Pe+ \\ IF+ \to R+ \\ Su+ \to B+ \\ P+ \to I+ \end{cases} \quad \rho_1 = \begin{cases} 1\to 1' \\ 2\to 2' \\ 3\to 3' \\ 4\to 4' \\ 5\to 5' \\ 6\to 6' \end{cases}$

   $S(\mu_1,\rho_1) = -12/24$

2. $\mu_2 = \begin{cases} PF+ \to Pe+ \\ IF+ \to I+ \\ Su+ \to R+ \\ P+ \to B+ \end{cases} \quad \rho_2 = \begin{cases} 1\to 3' \\ 2\to 5' \\ 3\to 1' \\ 4\to 4' \\ 5\to 2' \end{cases}$

   $S(\mu_2,\rho_2) = -3/24$

3. $\mu_3 = \begin{cases} PF+ \to B+ \\ IF+ \to I+ \\ Su+ \to R+ \\ P+ \to Pe- \end{cases} \quad \rho_3 = \begin{cases} 1\to 4' \\ 2\to 5' \\ 3\to 3' \\ 4\to 1' \\ 5\to 2' \end{cases}$

   $S(\mu_3,\rho_3) = 5/24$

The first pair of mappings is the trivial one, where we match entities and rules in the same order as they appear. In this case and as expected, the similarity score is rather low as there are only hazardous correspondences. The second and the third one have better scores and they are closer to the optimal solution that is discussed in the next section. The third matching suggests that birds and insects have the same role as piscivorous and insectivorous fish respectively, while the presence of the pond can be assimilated to the absence of pesticides. ◇

Ecosystems may be compared through the scoring function. In particular, if one of the ecosystems represents an interaction pattern we can search for it using the same method, as shown in Example 5.

Example 5. *Take the interaction pattern of predation in Table 3.*

The scores that we obtain for some mappings between the pattern above and the ecosystems from Examples 1 and 2 are given below.

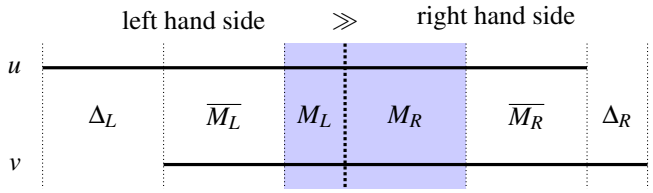


Figure 2: Schema of the scoring function for rules u and v represented as two horizontal lines; M_L and M_R are the matching parts of u and v; $\overline{M_L}$ and $\overline{M_R}$ are the parts which do not match while the length of the rules would allow to do so, and Δ_L and Δ_R are the parts which cannot match because of the different length of the rules.

1.

$$\mu_1 = \begin{cases} Pred+ \to Pe+ \\ Prey+ \to R+ \end{cases} \qquad \rho_1 = \begin{cases} 1'' \to 1' \\ 2'' \to 2' \end{cases}$$

$$S(\mu_1, \rho_1) = -4/6$$

2.

$$\mu_2 = \begin{cases} Pred+ \to Pe+ \\ Prey+ \to I+ \end{cases} \qquad \rho_2 = \begin{cases} 1'' \to 4' \\ 2'' \to 2' \end{cases}$$

$$S(\mu_2, \rho_2) = 2/6$$

3.

$$\mu_3 = \begin{cases} Pred+ \to B+ \\ Prey+ \to I+ \end{cases} \qquad \rho_3 = \begin{cases} 1'' \to 1' \\ 2'' \to 2' \end{cases}$$

$$S(\mu_1, \rho_1) = 4/6$$

One may observe that the third pair of mappings, having also the best score among the three matches, matches perfectly the entities and the rules, i.e., we may easily identify that B plays the role of the predator and I the role of the prey. It turns out that this is indeed an optimal solution, i.e., a pair of mappings that maximizes the scoring function. The second match also gives a good but less perfect score as rule $2''$ and 2 do not match on their outputs. Nevertheless, this second mapping suggests that pesticides, even if they are not living entities, may also be interpreted as predators. The first match is more arbitrary and as expected its score is also the lowest among the three matches. ◇

5 EXPERIMENT: SEARCHING PATTERNS INTO MODELS OF ECOSYSTEMS

In order to evaluate how practical our matching method is, we have implemented a prototype tool and used it to search patterns into various models of ecosystems. Both patterns and models are originated from previous works involving realistic ecosystem modeling. This tool performs the following steps that use the definition of scoring function given above:

1. Read models $\mathcal{E}_1$ of the pattern and $\mathcal{E}_2$ of the ecosystem in which the pattern is searched for.
2. Build the variables in matrices X and Y, and the scoring function $S(X,Y)$ as explained in the previous section.
3. Encode $S(X,Y)$ into a pseudo-Boolean optimization (PBO) problem following the requirements of the *competitions of pseudo-Boolean solvers* (Roussel and Manquinho, 2012, PB16, 2016).
4. Call a PBO solver and extract its solution. The solution can be interpreted back as the mappings of entities and rules that gives the best score.

As PBO solver, we have used Sat4j that appears to be quite fast and can be interrupted during its computation, in which case it proposes the best solution found so far. This is a very nice feature considering that searching for an optimal solution may be very long while non-optimal solutions may already correspond to interesting matches for the modeler. The prototype itself was implemented in Python using SymPy (SymPy development team, 2016) to build the scoring function as defined above and simplified to match the constraints of the PBO format.

This is illustrated in Figure 3 where we see how our prototype executes on the ecosystems from Examples 1 and 2: it prints the values of the scoring function as soon as Sat4j finds them. At any time, it is possible to kill Sat4j which interrupts its computation and force it to print the best solution it has discovered so far. It is interesting to note that this solution corresponds to none of those proposed in Example 4 which are all matches that have been crafted manually and corresponded to our intuition about the two models. So, this shows that our method is able to propose something new, i.e., something that a modeler would not necessarily imagine even on small examples.

5.1 Benchmark

Using this prototype, we have systematically searched for 12 patterns into 21 models of ecosystems. These

```
### reading 'pond.rr'
### 4 variables / 7 rules / 0 constraints
### reading 'pest.rr'
### 4 variables / 6 rules / 0 constraints
### building model
### running sat4j
... satisfiable [0:00:00.637612]
... objective function=2/24 [0:00:00.639101]
... objective function=4/24 [0:00:01.144709]
... objective function=6/24 [0:00:01.649645]
... optimum found
=== done running sat4j in 0:00:03.193784
*** OPTIMAL SAT => 6/24
### states
P+   ==>  Pe+
IF+  ==>  I+
Su+  ==>  R+
PF+  ==>  B+
### rules
R5: IF- >> PF-  ==>  R2: I- >> B-
R4: PF+ >> IF-  ==>  R1: B+ >> I-
R2: Su+ >> P-   ==>  R5: R+ >> Pe-
### normal exit
```

Figure 3: A sample run of our prototype searching matches between the Pond and Pesticides models presented in Examples 1 and 2.

patterns and models are all originated from various works performed by ecologists, in particular master students who have modeled contrasted ecosystems. The models are representation of ecosystems from the south of France (Camargue), the Alpes (Chamrousse) and ecosystems in Africa (Uganda, Karamoja). The patterns searched are mainly species interactions such as predation, competition, symbiosis, etc. It is out of the scope of this paper to describe these interactions, but we would like to pinpoint that they are all patterns and models that ecologists are actually interested in and not arbitrary examples. In particular, we did not include the "pond" and "pesticides" models in this benchmark, because they have been designed to illustrate this paper and have no ecological interest. For each search, we have defined a timeout of 3 minutes (180 seconds)[1] after which Sat4j was interrupted. Among the 252 searches resulting from this benchmark, 194 (77%) returned an optimal solution before the timeout, and 58 (23%) have been interrupted resulting in a non-optimal solution, as summarized in Figure 4. Even if the search time is short, we can observe that an optimal solution is found in most cases. For the other ones a solution, even if not optimal, is found anyway.

A more detailed view of this benchmark is provided in the "heat-map" depicted in Figure 5 that shows for each pattern and each model a color corresponding to the search time. In this heat-map, models are named with an upper-case letter, and patterns with a lower-case letter; names are followed by pairs of numbers e/r where e is the number of entities and r the number of rules in the model or pattern. For instance, the "prey-predator" and "live-in" patterns we have presented in the introduction are e and d respectively. Columns and rows have been sorted with respect to the sum of the values in the column and row, which allows to group larger search times in the lower-right corner. From this plot we can draw the following observations:

- neither patterns nor models size seem to be the key factor that lead to the significant search time increase. For instance, models S and J have very similar sizes but do not yield similar search times. The same remark applies to patterns e and g to j;
- however, the shape of the heat-map shows that a key factor lies in patterns as pattern choice may yield a significant increase of search time, while increasing is more progressive with respect to model choice;
- for toy models (A to F at the top), the solution is always quickly found;
- for large, more detailed, models (O to U at the bottom), the pattern structure is the key factor to determine if a timeout occurs;
- this is confirmed on intermediary models (G to N in the middle) where we can observe that more searches timeout as we go down the plot and, patterns all have the same size while models are not necessarily ordered by size.

So far, we have not identified what is the key factor that forbids a quick search. For sure pattern size is a factor as we can see for patterns k and l (or models O to U), but what we observe from patterns g—j and models F—L shows that this is not the only aspect. Considering our scoring function, search time is probably linked to the size of rules in the pattern and in the model, but this question will deserve further work to examine more in depths the characteristics of patterns that lead to the observed increasing of search times.

As a conclusion of this benchmark, we observe that searching a pattern in a model is always possible, usually in a very short time. Moreover, in every case, a solution has been found quickly, which allows the user to interrupt the search very soon and yet get a match that is not optimal with respect to the scoring function but may be interesting already.

A future extension of the implementation would be to enable re-injecting found matches in the PBO problem as negative constraints, in order to forbid the

[1] The choice of 3 minutes is arbitrary.

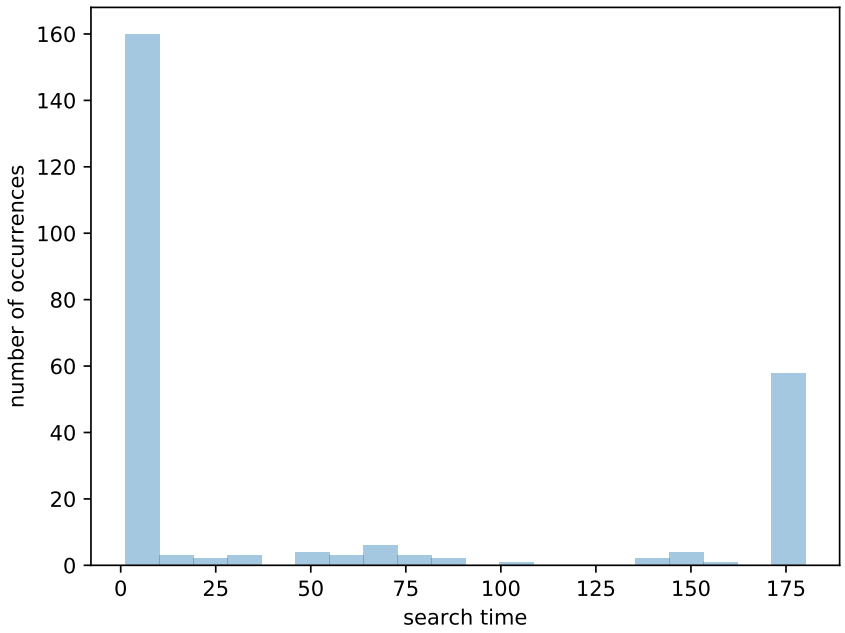


Figure 4: Histogram of search times (in seconds) in the benchmark.

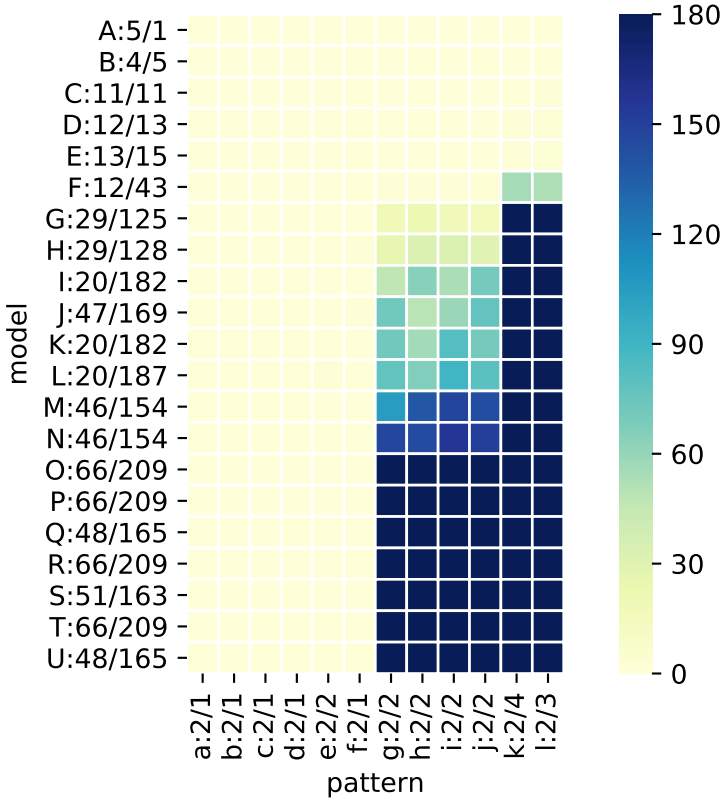


Figure 5: Search times (in seconds) with respect to models and patterns. Models are indicated with an upper-case letter, patterns with a lower-case letter. Model and pattern names are followed by pairs of numbers e/r: e is the number of entities and r the number of rules.

search to find them again. In addition, this would give a way to enumerate matches. It is indeed particularly relevant for ecologists to (automatically) identify several instances of the same interaction pattern (ecological processes) in the ecosystem dynamics under study.

6 CONCLUSION AND PERSPECTIVES

In this paper, we have presented a method for automatically comparing and assessing similarity between ecosystems defined as specific kinds of rewriting systems. We have defined a scoring function that takes into account not only the number of matching entities and rules, but also the quality of partial mappings between the left and right hand sides of rules. The approach has been successfully applied to the search of known interaction patterns (i.e., ecological processes) in models of ecosystems.

The results we have obtained in our benchmark are promising: we quickly obtain optimal solutions for the vast majority of the cases studied. For the remaining ones, we obtain a solution that is not optimal in a short time, but we have no assessment of how far from optimal it is. A possible option to solve this issue could be to add ecological information to assess the quality of a match (with a relevance score) closer to the modeler's expectations. In other words, a bigger match is not necessarily a better match. So far, our method searches for bigger matches. When the search is interrupted and yields to a sub-optimal solution, a relevance score may help deciding whether it is already a "good" match or not. In practice, the matching of entities (here, ecosystemic entities) and rules (ecological processes) can be guided by adding additional constraints, such as to:

- enforce the matching/identity between subsets of entities or rules. For example, if the model allows different categories of rules (each category possibly having a different semantics), the scoring function could be adapted to take into account this extension;
- enforce the matching between entities/rules of the same category (for example match carnivores among them);
- diminish the importance of some entities/rules (i.e., set a different weight for each matching up to forget some, if necessary).

Finally, as a long term perspective, we may use our method to discover invariant patterns that are not known in advance, thus increasing the understanding about ecosystem functioning. This could account for using our concept of similarity to identify matching parts of ecosystems and extract from those the new patterns. Experiments we have conducted so far in this direction showed bad performances as search time becomes prohibitive (as if we would have used patterns whose sizes are close to the studied models' sizes). However, sub-optimal patterns may provide interesting matches (which remains to be studied), or we may find a way to guide the search with respect to additional constraints (related to the previous idea of a relevance score).

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REFERENCES

Agnihotri, K. and Sharma, N. (2015). Developments in ecological modeling based on cellular automata. 6.

Bae, J., Liu, L., Caverlee, J., and Rouse, W. B. (2006). Process mining, discovery, and integration using distance measures. In *2006 IEEE International Conference on Web Services (ICWS'06)*, pages 479–488.

Baldan, P., Bocci, M., Cocco, N., and Simeoni, M. (2013a). Comparing metabolic pathways through potential fluxes: a selective opening approach. In *BioPPN@Petri Nets*.

Baldan, P., Cocco, N., Giummolè, F., and Simeoni, M. (2013b). Comparing metabolic pathways through reactions and potential fluxes. *Trans. Petri Nets and Other Models of Concurrency*, 8:1–23.

Baldan, P., Cocco, N., Marin, A., and Simeoni, M. (2010). Petri nets for modelling metabolic pathways: a survey. *Natural Computing*, 9(4):955–989.

Cardelli, L. (2005). Abstract machines of systems biology. *Transactions on Computational Systems Biology*, 3737:145–168.

Danos, V. and Laneve, C. (2004). Formal molecular biology. *TCS*, 325(1):69–110.

Delaplace, F., Di Giusto, C., Giavitto, J., and Klaudel, H. (2018). Activity networks with delays an application to toxicity analysis. *Fundamenta Informaticae*, to appear.

Dijkman, R., Dumas, M., van Dongen, B., Käärik, R., and Mendling, J. (2011). Similarity of business process models: Metrics and evaluation. *Information Systems*, 36(2):498 – 516. Special Issue: Semantic Integration of Data, Multimedia, and Services.

Ehrenfeucht, A. and Rozenberg, G. (2007). Reaction systems. *Fund. Inform.*, 75(1-4):263–280.

Euzenat, J. and Shvaiko, P. (2007). *Ontology Matching*. Springer-Verlag New York, Inc., Secaucus, NJ, USA.

Fages, F. and Soliman, S. (2008). Formal cell biology in biocham. In *Proceedings of the Formal Methods for the Design of Computer, Communication, and Software Systems 8th International Conference on Formal Methods for Computational Systems Biology*, SFM'08, pages 54–80, Berlin, Heidelberg. Springer-Verlag.

Gaucherel, C. (2006). Influence of spatial patterns on ecological applications of extremal principles. *Ecological Modelling*, 193:531–542.

Gaucherel, C., Boudon, F., Houet, T., Castets, M., and Godin, C. (2012). Understanding patchy landscape dynamics: Towards a landscape language. *PLoS ONE*, 7(9):16.

Gaucherel, C., Houllier, F., AUCLAIR, D., and Houet, T. (2014). Dynamic Landscape Modelling : The Quest for a Unifying Theory. *Living reviews in landscape Research*, 8(2):5–31.

Gaucherel, C. and Pommereau, F. (2017). Using Petri nets to identify basins of attraction and tipping points of an ecosystem. *submitted*.

Giavitto, J.-L., Malcolm, G., and Michel, O. (2004). Rewriting systems and the modelling of biological systems. *Comparative and Functional Genomics*, 5:95–99.

Grafahrend-Belau, E., Schreiber, F., Heiner, M., Sackmann, A., Junker, B. H., Grunwald, S., Speer, A., Winder, K., and Koch, I. (2008). Modularization of biochemical networks based on classification of Petri net t-invariants. *BMC Bioinformatics*, 9(1):90.

Henkel, R., Hoehndorf, R., Kacprowski, T., Knüpfer, C., Liebermeister, W., and Waltemath, D. (2018). Notions of similarity for systems biology models. *Briefings in Bioinformatics*, 19(1):77–88.

Le Berre, D. and Parrain, A. (2010). The Sat4j library, release 2.2. *Journal on Satisfiability, Boolean Modeling and Computation*, 7.

Lotka, A. J. (1925). *Elements of physical biology*. Williams & Wilkins Company, Baltimore.

May, R. M. (1972). Will a large complex system be stable? *Nature*, 238:413 EP –.

Milo, R., Shen-Orr, S., Itzkovitz, S., Kashtan, N., Chklovskii, D., and Alon, U. (2002). Network motifs: Simple building blocks of complex networks. *Science*, 298(5594):824–827.

Mooiman, L. (2015). Comparing stories with the use of Petri nets. Technical report, University of Amsterdam.

Paun, A., Paun, M., Rodríguez-Patón, A., and Sidoroff, M. (2011). P systems with proteins on membranes: a survey. *Int. Journal of Foundations of Computer Science*, 22(1):39–53.

PB16 (2016). Pseudo-Boolean competition 2016. `http://www.cril.univ-artois.fr/PB16`. Satellite event of SAT'16.

Roussel, O. and Manquinho, V. (2012). Input/output format and solver requirements for the competitions of pseudo-Boolean solvers. `http://www.cril.univ-artois.fr/PB12/format.pdf`.

Sangiorgi, D. (2011). *Introduction to Bisimulation and Coinduction*. Cambridge University Press, New York, NY, USA.

SymPy development team (2016). SymPy. `http://www.sympy.org`.

Terese (2003). *Term Rewriting Systems*, volume 55 of *Cambridge Tracts in Theoretical Computer Science*. Cambridge University Press.

Thomas, R. (1973). Boolean formalisation of genetic control circuits. *Journal of theoretical biology*, 42:565–583.

Tversky, A. (1977). Features of similarity. *Psychological Review*, 84(4):327–352.

van Glabbeek, R. and Goltz, U. (1989). Equivalence notions for concurrent systems and refinement of actions. In Kreczmar, A. and Mirkowska, G., editors, *Mathematical Foundations of Computer Science 1989*, pages 237–248, Berlin, Heidelberg. Springer Berlin Heidelberg.

Wang, J., He, T., Wen, L., Wu, N., ter Hofstede, A. H. M., and Su, J. (2010). A behavioral similarity measure between labeled Petri nets based on principal transition sequences. In *On the Move to Meaningful Internet Systems: OTM 2010 - Confederated International Conferences: CoopIS, IS, DOA and ODBASE, Hersonissos, Crete, Greece, October 25-29, 2010, Proceedings, Part I*, pages 394–401.

Xiao, L., Zheng, L., Xiao, J., and Huang, Y. (2009). A graphical query language for querying Petri nets. In Yang, J., Ginige, A., Mayr, H. C., and Kutsche, R.-D., editors, *Information Systems: Modeling, Development, and Integration*, pages 514–525, Berlin, Heidelberg. Springer Berlin Heidelberg.