Mathematical Morphology on Soft Sets for Application to Metabolic Networks

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Abstract. In this paper, we introduce mathematical morphological operators such as dilation and erosion on soft sets. Rather than the common approach which is based on expressing soft set analogues of the classical theory, we use the classical theory to morphologically analyse a soft set. The main goal of our study is to apply this morphological concepts to metabolic networks to derive an algebraic picture of chemical organizations. For this purpose we first introduce various types of complete lattices on soft sets which represent metabolic networks, then study morphological operations respect to corresponding lattice structure. We also give the concept of duality on soft sets.

1 Introduction

Soft set theory, introduced by Molodtsov in [4], is a mathematical tool for dealing with uncertainty of real world problems that involve data which are not always crisp. It differs from the theories of same kind like fuzzy sets theory, vague sets theory, and rough sets theory by the adequacy of the parametrization. Basically, a soft set over an initial universe set U is a pair (F, A), where F is a mapping $F : A \subset E \to P(U)$, E is a set of parameters, and $P(U)$ is the power set of the universe set. One may conclude that a soft set over U is a parameterized family of subsets of the universe U. Mathematically, a soft set is just a set-valued function mapping elements of a "parameter space" to subsets of a universe; alternatively, it can also be seen as a relation between these sets. Similar settings have been studied in a multitude of other fields. A striking example is Formal Concept Analysis [2]. In Formal Concept Analysis, the point of departure is a binary relation R between objects Y and properties X. From such a relation, one can of course construct set-valued functions, for example a function mapping a property x to the subset of objects y such that $R(x, y)$, i.e., those objects having property x; formally, this corresponds exactly to the soft set representation. However, the other way around, one can also map an object y to the subset of properties it has, i.e., to the subset of x such that $R(x, y)$. Formal Concept Analysis is looking at these mappings simultaneously and constructing so-called formal concepts from this. For the sake of simplicity, we prefer the analysis of soft sets which involves the more simple structure. It can be also seen that a soft set is not a set but set systems. By the arise of the theory its algebraic [9, 35] and topological [34] properties, its relation with other theories [7, 31, 33], and also implicational feature of the theory [8, 29, 30] have been studied intensively. We refer [25] to the interested readers for soft set theoretical analogues of the basic set operations. Throughout this paper we will denote the sets of soft sets over the universe U as $S(U)$, and the image of a subset of the parameter set under the mapping F as $F(A)$.

Mathematical Morphology is a well-founded and widely used non-linear theory for information processing. It has started by analysing set of points with certain kinds of set theoretical operations like Minkowski sum and Minkowski substraction [19, 23], then with the development of information systems, it was necessary to generalize set theoretical notions to complete lattices [3, 6, 10, 17]. Beside the general fashion to use mathematical morphology in image and signal processing, it also finds application areas in topology optimization [32], spatial reasoning [15, 16], preference modeling and logics [13, 14]. Extending mathematical morphology to soft set theory will increase the modeling and reasoning in all these areas. This extension can be performed by defining complete lattices as the underlying structure of soft sets, and then lead us the definitions of algebraic dilations and erosions.

Organization and functioning of metabolic processes is a subject of biochemistry that still has lots of research attention by the new opportunities to study the mechanisms and interactions that govern metabolic processes. Algebraic approaches to chemical organizations in terms of set-valued set-functions that encapsulate the production rules of the individual reactions lead us to mathematically define generalized topological spaces on the set of chemical species. From the mathematical point of view, these approaches mostly depend on the kinetic models and topological network analysis, with their own benefits [1, 5, 11, 18, 24, 26–28]. Topological network analysis does not have to suppose any knowledge of kinetic parameters, therefore is a useful mathematical tool for less well characterized organisms. It is also applicable to complex systems such as chemical reaction networks. Therefore it allows us to study topological properties with less computational complexities.

In this study, we consider morphological operations on soft sets which are set systems with various application benefits to metabolic networks. In Section 2, we introduce certain kinds of complete lattices that can be constructed on a soft set. Rather than straightforward ones, we define the complete lattices involving information about both universe and parameter set. In Section 3, we study the basic morphological operators like dilation and erosion on soft sets. And by the trivial decompositions of soft sets, we give the idea of structuring element for a soft set. In Section 4, we present the soft set model and the mathematical morphological operations of the KEGG [22] representation of the cysteine metabolism network in P.fluorescens PfO-1. For the sake of clarifying the method, we consider trivial lattices in this model. These lattices can be extended to the other ones and different structuring elements can be obtained. In

Section 5, we introduce the concept of the dual of a soft set and study this idea with respect to morphological dilations.

2 Lattice Structures on Soft Sets

A classical lattice structure on the universe set may be defined directly by $\mathcal{L}_U = (P(U), \subseteq)$ where $P(U)$ is the power set of the universe set. Since this lattice do not involve the complete information about the soft set, it may not be useful. To take the parameter sets into the account we may define more useful lattice structure as follows.

Definition 1. *Let (F, A) be a soft set and $x \in U$. Degree of a point is the number of parameters assigned by F to x denoted by $d(x)$. If $H(x) = \{a \in A \subset E \mid x \in F(a)\}$, then $d(x) = s(H(x))$.*

Definition 2. *Let (F, A) be a soft set and $U' \subseteq U$. If for all $(x, y) \in U' \times U$ $F(H(x) \cap H(y)) \subseteq U'$, then we say U' is a closed universe set. We denote the family of closed sets by $\mathcal{C}(U)$.*

Remark 1. It's straightforward to see that $\emptyset \in \mathcal{C}(U)$.

Proposition 1. *The structure $(\mathcal{C}, \subseteq)$ is a complete lattice with for all $(V', V'') \in \mathcal{C}(U) \times \mathcal{C}(U)$*

$$V' \wedge V'' = \cup\{V''' \in \mathcal{C}(U) \mid V''' \subseteq V' \cap V''\}$$

is the infimum and

$$V' \vee V'' = \cap\{V''' \in \mathcal{C}(U) \mid V' \cup V'' \subseteq V'''\}$$

is the supremum.

A complete lattice on the power set of the parameter set A can be defined directly by $\mathcal{L} = (P(A), \subseteq)$. One may apply classical lattice results here directly. However, the next lattice definitions are noteful since they also involve information about the universe set.

Definition 3. *Let (F_1, A_1) and (F_2, A_2) be two soft sets over $U_1 \subseteq U$ and $U_2 \subseteq U$ respectively. A partial order $\preceq$ can be defined as*

$$(F_1, A_1) \preceq (F_2, A_2) \iff U_1 \subseteq U_2,\ A_1 \subseteq A_2.$$

Proposition 2. *$(S(U), \preceq)$ is a complete lattice. It's infimum is*

$$(F_1, A_1) \wedge (F_2, A_2) = (U_1 \cap U_2, A_1 \cap A_2)$$

and for any family $\bigwedge_i (F_i, A_i) = (\bigcap_i U_i, \bigcap_i A_i)$. It's supremum is $(F_1, A_1) \vee (F_2, A_2) = (U_1 \cup U_2, A_1 \cup A_2)$ and for any family $\bigvee_i (F_i, A_i) = (\bigcup_i U_i, \bigcup_i A_i)$.

Definition 4. *Let (F, A) be a soft set over the universe U. (F, B) is an induced soft subset of (F, A) if $B = \{b_i \in U \mid b_i = F(a_i), a_i \in A\}$ for $i \in \{1, 2, \ldots\}$.*

Definition 5. *Let (F, A) be a soft set over the universe U and (F, A_1) and (F, A_2) are induced soft subsets of (F, A). A partial order $\preceq_{in}$ can be defined as*

$$(F, A_1) \preceq_{in} (F, A_2) \iff A_1 \subseteq \{F(a) \cap U \mid a \in A_2\}.$$

Proposition 3. *$(S(U), \preceq_{in})$ is a complete lattice with the infimum*

$$(F, A_1) \wedge_{in} (F, A_2) = (F, \{F(a_1) \cap F(A_2), F(a_2) \cap F(A_1) \mid a_1 \in A_1, a_2 \in A_2\})$$

and the supremum

$$(F, A_1) \vee_{in} (F, A_2) = (F, A_1 \cup A_2).$$

The smallest element of the lattice is the null soft set.

Definition 6. *Let I be the set of isomorphism classes of soft sets, and . A partial order $\preceq_f$ on I can be defined as*

$$(F_1, A_1) \preceq_f (F_2, A_2) \iff (F_1, A_1) \text{ is isomorphic to an induced soft subset of } (F_2, A_2) \text{ by } f$$

3 Morphological Operators on Soft Sets

Let $(\mathcal{L}, \preceq)$ and $(\mathcal{L}', \preceq')$ be two complete lattices.

Definition 7. *An operator $\delta : \mathcal{L} \to \mathcal{L}'$ is a dilation on a soft set (F_i, A_i) for $i \in \{1, 2, \ldots\}$ if*

$$\forall (F_i, A_i) \in \mathcal{L},\ \delta(\vee_i (F_i, A_i)) = \vee'_i \delta(F_i, A_i)$$

where $\vee$ and $\vee'$ denote the supremums to $\preceq$ and $\preceq'$,respectively. Similarly, an operator $\epsilon : \mathcal{L}' \to \mathcal{L}$ is a erosion on a soft set (F_j, A_j) for $j \in \{1, 2, \ldots\}$ if

$$\forall (F_j, A_j) \in \mathcal{L}',\ \epsilon(\wedge_j (F_j, A_j)) = \wedge'_j \delta(F_j, A_j)$$

where $\wedge$ and $\wedge'$ denote the infimums to $\preceq$ and $\preceq'$,respectively.

In mathematical morphology, an essential part of the dilation and erosion operations is the structuring element which allows us to define arbitrary neighborhood structures. Structuring element can be interpreted as a binary relation between two elements. Therefore, it is possible to extend this idea to any lattice. Generally, the structuring element of x is defined as $B_x = \delta(\{x\})$, where x can be element of the universe set or the parameter set. Hence, it is directly depended on the definition of the corresponding dilation. Just before clarify this idea with an example, we would like to introduce canonical decomposition of a soft set with respect to considered lattice.

For the lattice $(P(U), \subseteq)$, trivial decomposition of each subset of the universe set U is $U = \bigcup_{x \in U} \{x\}$ and its corresponding morphological dilation is $\bigcup_{x \in U} B_x = \bigcup_{x \in U} \delta(\{x\})$. In the same sense, for the lattice $(P(E), \subseteq)$, trivial decomposition of each subset of the parameter set E is $E = \bigcup_{a\in E}\{a\}$ and its corresponding morphological dilation is $\bigcup_{a\in E} B_a = \bigcup_{a\in E} \delta(\{a\})$. Let us now consider a complete lattice structure defined on a soft set (F, A) as Definition 3. For A, a natural decomposition is $A = \bigvee_{a\in A}\{a\}$. For the decomposition of U, we need a reliable one with the assignment of the parameters. Hence, for $U^{\emptyset} = \{x \in U \mid x \notin F(A)\}$,

$$(F, A) = \left(\bigvee_{a\in A} (F(a), \{a\})\right) \vee \left(\bigvee_{x\in U^{\emptyset}} (\{x\}, \emptyset)\right)$$

is the canonical decomposition of a soft set. The other types of canonical decompositions respect to given lattice structure on the soft set can be obtained by following the same procedure.

4 Mathematical Morphology on Metabolical Networks

Directed graphs are main mathematical tools to represent metabolic networks [12, 20, 21]. In this representation, metabolites are nodes and an arc corresponds to the state of being a reaction between any two metabolites. Since a common reaction have more than one substrate and/or product, and any two metabolites may be involved by more than one reaction, directed graph representation of a metabolic network gets being handicapped. To handle this problem, we propose soft set representation of such metabolic networks.

Let us consider the standard representation of the cysteine metabolism network in *P.fluorescens* PfO-1 in Figure 1. One reads the soft set representation of this network as:

$F_{out}(R00568) = \{C00010, C00024, C00065, C00979\}$ $F_{out}(R00590) = \{C02218\}$
$F_{out}(R01874) = \{C00014, C00022, C00283\}$ $F_{out}(R03132) = \{C00033, C05824\}$
$F_{out}(R04859) = \{C00033, C00097, C00343, C00094\}$ $F_{out}(R03650) = \{C00013, C03125\}$
$F_{out}(R02433) = \{C00026, C00302, C00506, C05528\}$ $F_{out}(R00896) = \{C00010, C00097\}$
$F_{out}(R02619) = \{C00302, C05527\}$ $F_{out}(R04861) = \{C00029, C05532\}$
$F_{out}(R03105) = \{C00094, C00957\}$ $F_{out}(R00897) = \{C00033, C00097\}$
$F_{out}(Null) = \{C00022\}$

$F_{in}(R00568) = \{C00010, C00024, C00065, C00979\}$ $F_{in}(R00590) = \{C00065\}$
$F_{in}(R01874) = \{C00097\}$ $F_{in}(R03132) = \{C00320, C00979\}$
$F_{in}(R04859) = \{C00320, C00342, C00979\}$ $F_{in}(R03650) = \{C00097, C01639\}$
$F_{in}(R02433) = \{C00026, C00302, C00506, C05528\}$ $F_{in}(R00896) = \{C00302, C00957\}$
$F_{in}(R02619) = \{C00026, C00606\}$ $F_{in}(R04861) = \{C05527\}$
$F_{in}(R03105) = \{C05529\}$ $F_{in}(R00897) = \{C00283, C00979\}$
$F_{in}(Null) = \{C05529\}$

with F_{out} and F_{in} parameter mappings that defined on the set of biochemical reactions R to the universe set of metabolites M. More precisely, F_{out} and F_{in} maps the corresponding biochemical reaction to the produced and substrate metabolites, respectively. Moreover, by adding a null reaction to the R, this mapping

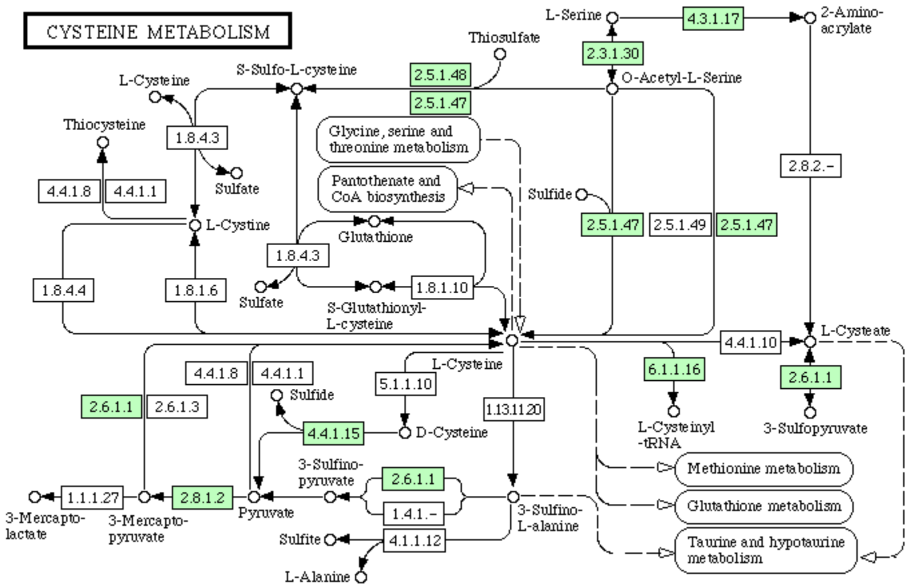

Fig. 1. A standard representation of the cysteine metabolism network in P. fluorescens PfO-1 from KEGG [22].

becomes well-defined. The reader also shall note that the compounds such as ATP, AMP, and H_2O are not considered in the soft sets (F_{in}, R) and (F_{out}, R). We also use the corresponding abbreviations of the reactions and compounds respect to KEGG database [22] for the improve readability.

Let us now consider the complete lattice $\mathcal{L} = (P(M), \subseteq)$. Now consider structuring elements of dilation on biochemical reaction set:

$$\forall a \in R,\ B_a = \delta(\{a\}) = \{a' \in M \mid F_{out}(a) \cap F_{in}(a') \neq \emptyset\}$$

and then applying these morphological dilations, one may obtain following results:

$$\begin{array}{ll} B_{R00568} = \{R00568, R00590, R00897\} & B_{R00896} = \{R00568, R00590, R00897\} \\ B_{R04859} = \{R01874, R03650\} & B_{R02433} = \{R00896, R02433\} \\ B_{R00897} = \{R01874, R03650\} & B_{R01874} = \{R00897\} \\ B_{R03105} = \{R00896\} & \end{array}$$

Another dilation can be defined on reactions to the universe of metabolites as

$$\forall a \in R,\ B'_a = \cup \{F_{in}(a') \mid F_{out}(a) \cap F_{in}(a') \neq \emptyset\},$$

and then the dilation reads

$$\begin{aligned}
B'_{R00896} &= \{C00010, C00024, C00065, C00097, C00979, C01639\} \\
B'_{R00568} &= \{C00010, C00024, C00065, C00213, C00979\} \\
B'_{R02433} &= \{C00026, C00302, C00506, C00957, C05528\} \\
B'_{R01874} &= \{C00283, C00979\} \\
B'_{R03105} &= \{C00302, C00957\} \\
B'_{R00897} &= \{C00097, C01639\}.
\end{aligned}$$

5 Morphological Dilation Dualities

Definition 8. *Let (F, A) be a soft set with non-empty parameter and universe set. The dual of the soft set (F, A) is defined with $F^* : A^* \subset U \to E$, where U is the universe set and E is the parameter set of (F, A) and denoted by (F^*, A^*).*

Remark 2. One may conclude by the definition that the dual of two isomorphic soft sets are also isomorphic to each other.

Now, let $\delta : U \to P(U)$ be a mapping and its dual be a mapping $\delta^* : U \to P(U)$ defined as $\delta^*(\{x\}) = \{y \in U \mid x \in \delta(\{y\})\}$. It also follows that $\delta^{**} : U \to P(U)$, $\delta^{**}(\{x\}) = \{y \in U \mid x \in \delta^*(\{y\})\}$.

Theorem 1. *Let (F, A) be a soft set over the non-empty universe set and $A \neq \emptyset$. $\forall V \in P(U)$*

1. *$\delta^*(V) = \bigcup_{x \in V} = \{y \in U \mid V \cap \delta(\{y\}) \neq \emptyset\}$ iff δ^* is a dilation.*
2. *$\bigcup_{x \in V} \delta^*(\{x\}) = U$ implies that $V \subseteq \bigcup_{V \cap \delta^*(\{y\}) \neq \emptyset} \delta^*(\{y\})$.*
3. *On the universe set U, $\delta^{**} = \delta$.*

Proof. 1. *If δ^* is a dilation, then it is straightforward by the definition. Now let us consider $y \in \delta^*(V)$ for $V \in P(U)$, then there exists $x \in V$ such that $y \in \delta^*(x)$ iff $x \in \delta(\{y\})$. Therefore, $y \in \{z \in U \mid V \cap \delta(\{z\}) \neq \emptyset\}$. Now, let $V \in P(U)$ and $y \in \{z \in U \mid V \cap \delta(\{z\}) \neq \emptyset\}$, then there exists $x \in V$ such that $x \in \delta(\{y\})$ iff $y \in \delta^*(\{x\})$. This implies $y \in \bigcup_{x \in V} \delta^*(\{y\})$. Conversely, if the equalities hold, since δ^* commutes with the supremum, δ^* is a dilation.*
2. *Straightforward*
3. *Let $z \in \delta^{**}(\{x\})$. This implies that $x \in \delta^*(\{z\})$, hence $z \in \delta(\{x\})$. Similarly, $z \in \delta(\{x\})$ implies that $x \in \delta^*(\{z\})$, therefore $z \in \delta^{**}(\{x\})$.*

One of the significant results arise with the choose of parameter map as the structuring element. Let $\delta : P(U) \to P(U)$ be a dilation. Then, for $x \in U$, $(F, A)_\delta = (\delta(\{x\}), A)$ is a soft set. We can also define a dilation to any soft set (F, A) by considering the structuring element as $\delta : V \to P(A)$, $\delta(\{x\}) = \{a \in A \mid x \in F(a)\}$. These ideas lead us to following theorem:

Theorem 2. *Let $\delta : U \to P(U)$ be a mapping and (F, A) be a soft set with the bijective parameter map. Then, (F, A) is isomorphic to $(F, A)_\delta$ iff (F^*, A^*) is isomorphic to $(F, A^*)_{\delta^*}$.*

Proof. *Let (F, A) and $(F, A)_\delta$ be two isomorphic soft sets. By the definition of dilation, if $x \neq y$ then $\delta(\{x\}) \neq \delta(\{y\})$, that is $\delta(\{x\}) = \delta(\{y\})$ implies that $x = y$. Therefore, δ is injective on U.*

Moreover, by the isomorphism there exists a bijection $f : (F, A) \to (F, A)_\delta$ such that $a \in A$ iff for $x \in U$, $f(a) = \delta(\{x\}) \in A_\delta$. Notice that $A_\delta = \{\delta(\{x\}),\ x \in U\}$.

Let (F^*, A^*) be a dual of (F, A). (F^*, A^*) is a soft set over the universe U^*. By the definition of the duality, U^* is isomorphic to A and A^* is isomorphic to U. Hence, (F, A) is isomorphic to $(F, A)_\delta$ iff (F^*, A^*) is isomorphic to $(F^*, A^*)_\delta$.

Now it is sufficient to show that $(F^*, A^*)_\delta$ is isomorphic to $(F, A^*)_{\delta^*}$. Here, $(F^*, A^*)_\delta$ is the soft set with U^*_δ is isomorphic to A_δ and A^*_δ is isomorphic to $H^*(x) = \{u \in A^* \subset U \mid x \in F^*(u)\}$.

Let $g : \{\delta(\{y\}), y \in U\} \to U$ defined by $g(\delta(\{y\})) = y$. g is well defined, since $\delta(\{x\}) = \delta(\{y\}) \implies g(\delta(\{x\})) = g(\delta(\{y\}))$ for $x = y$.

It can be clearly seen that g is surjective; and by the equality of the cardinalities of $\{\delta(\{y\}), y \in U\}$ and U, g is injective.

Now, $H^*(x) \in A^*_\delta$ iff $H^*(x) = \{\delta(\{u_i\}), x \in \delta(\{u_i\})\} \in A^*_\delta$ iff $g(H^*(x)) = \{g(\delta(\{u_i\})), i \in \{1, 2, \ldots, n\}\} = \{u_1, u_2, \ldots, u_n\} = \delta^*(\{x\})$; since $x \in \delta(u_i)$ iff $u_i \in \delta^*(\{x\})$. Therefore, $(F^*, A^*)_\delta$ is isomorphic to $(F, A^*)_{\delta^*}$.

6 Conclusions

In this paper, we introduced mathematical morphology on soft sets. To obtain the morphological operations such as dilation and erosion, we studied some introductive complete lattices on soft sets. While constructing these lattices, we consider the cases where information about parameters and universe is preserved. By the help of complete lattices, we were able to define morphological operations and the structuring element. A new duality definition for the soft set theory was also given to show the relevance of relationship between mathematical morphology and soft sets.

The morphological interpretation of metabolic networks led us to derive an algebraic picture of chemical organizations. By the discontinuous nature of the metabolic networks, we need to state this new approach to define concepts such as connectedness, similarity, and continuity of change. For the representation of the cysteine metabolism network in P. fluorescens PfO-1, it is possible to obtain such concepts by the help of mathematical structuring element. We may also conclude from our analysis that the reactions $R00590, R03132, R03650, R04861$, and $Null$ do not have any dilations. Different structuring elements also lead us to obtain different morphological characteristic of the network. For instance, by new structuring element

$$\forall a \in R,\ B_a^k = \delta(\{a\}) = \{a' \in R \mid |F_{out}(a) \cap F_{in}(a')| \geq k\},$$

where $|,|$ denotes the maximum cardinality, it can be seen that only $R00586$ and $R02433$ have the stronger connectedness for $k \geq 2$. Different kinds of structuring elements which may be more suitable for the model under consideration can be obtained by choosing different lattices on soft sets.

Authors' contributions

Mehmet Ali Balcı and Ömer Akgüller worked together in the derivation of the mathematical results. Both authors read and approved the final manuscript.

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