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A creative abduction approach to scientific and knowledge discovery

H. Prendinger[a,*], M. Ishizuka[b]

[a]National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan
[b]Department of Information and Communication Engineering, Graduate School of Information Science and Technology, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

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Abstract

In this paper we explore the range of applicability of abductive reasoning for knowledge discovery. In particular, we discuss a novel form of abduction, called *creative* abduction, where new knowledge is generated in the process of explaining observed events, and demonstrate its relevance to knowledge discovery. The main contribution of this paper is twofold: *First*, we show that creative abduction can be used to infer a disposition explaining local temporal regularities. In the presence of multiple correlated regularities, this form abduction may significantly unify a given corpus of knowledge, corresponding to theory formation in scientific discovery. *Second*, we present a weaker form of creative abduction that infers a goal (e.g. interest) from simple 'condition-effect' rules called 'transitions'. If multiple transitions are correlated, the weaker form of creative abduction can be used to identify, e.g. clusters of Web users, as done in Web usage mining. We will focus on the formal underpinnings of this new form of abduction that seems readily applicable to a wide range of practical knowledge discovery problems.

Keywords: Abduction; Logic for knowledge discovery; Scientific discovery

1. Introduction

We take the notion of 'knowledge discovery in databases' (KDD) to mean methods that generate new, plausible, useful, and intelligible knowledge for observed events. Similar definitions can be found in the literature, differing mostly in emphasizing individual features of the produced knowledge [2,17].

In this paper, we advocate an approach to knowledge discovery that is based on *abductive* reasoning, an inference scheme originally introduced by Peirce [10]. The standard formulation describes abduction as an inference to a hypothesis C that would explain the evidence E, given the law $E \leftarrow C$. This form of abduction became a prevalent reasoning mechanism in many fields of artificial intelligence such as diagnosis, natural language understanding, default reasoning, database updates, planning, and high-level vision [5,7,12,13]. From a knowledge discovery point of view, however, the standard form of abduction is rather uninteresting since in principle, all the knowledge needed to explain the observations is already given in the problem formulation.

Schurz [15] observed that Peirce actually introduced two forms of abductive inference: the first one that he calls *non-creative* corresponds to the scheme mentioned above. The second form of abduction infers a *disposition* of certain objects that would explain a set of local temporal (empirical) regularities involving those objects. For instance, the hypothesis that a has the disposition of (electric) conductivity explains the local temporal regularity 'whenever object a is subject to a voltage source, a conducts current'. Since the predicate denoting the disposition is not already part of the theory, he calls this form of reasoning *creative* abduction. In addition to the abduced disposition, a new rule is inferred expressing that the set of empirical regularities is 'caused' by the objects' disposition. In order to state a causal relationship, the hypothesized disposition is also required to *unify* a given corpus of knowledge, which means that the abduced disposition can explain a set of *correlated* regularities.

The creative form of abduction can be used to accomplish many kinds of knowledge discovery tasks. In this paper, we will explore two such tasks. The first one is *scientific discovery* where a disposition (or cause) is invented to explain

* Corresponding author. Tel.: +81 3 4212 2650; fax: +81 3 3556 1916.
E-mail address: helmut@nii.ac.jp (H. Prendinger).

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multiple correlated empirical regularities. The second one employs a weaker form of creative abduction that is broadly applicable to KDD tasks, such as *Web usage mining* [3].

The rest of the paper is organized as follows. In Section 2, creative forms of abduction found in the literature are discussed. Section 3 is devoted to introducing disposition-creative abduction and its application to scientific discovery. In Section 4, goal-creative abduction, a weaker form of disposition-creative abduction, is introduced and its relevance to Web usage mining is demonstrated. Section 5 discusses related work, and Section 6 concludes the paper.

2. Related work

In this section, we offer a short primer on abductive reasoning, and discuss two forms of abduction found in the literature that can be called *creative* since some 'new' hypothesis is invented to explain observed events. There, a *new* hypothesis is a piece of knowledge that comes in two different syntactic forms:

- *Element-creative abduction*. The hypothesis is a constant denoting an hitherto unknown object (element) of the domain. Element-creative abduction is a method for scientific discovery, i.e. theory (or world model) revision, as it occurs in scientific revolutions [8].
- *Rule-creative abduction*. The hypothesis is a rule denoting a law that summarizes the given observations. This form of abduction is well-known as *inductive logic programming* (ILP) [6].

While element-creative abduction is an extension of the standard form of abduction, rule-creative abduction is an independent research field.

2.1. Element-creative abduction

In element-creative abduction, an *unknown object* of the domain is hypothesized to explain the observations. This form of abduction employs the standard (non-creative) definition of abduction. A *standard abduction problem* is characterized by a set of observations $\mathcal{O}$ ('effects') to be explained, given a logical theory Σ modeling some domain. An *abductive solution* to an abduction problem is a set of hypotheses which, if assumed, would explain the effects. The set of hypotheses H is typically restricted to some set $\mathcal{H}$ of 'assumable' predicates. More formally, an standard abductive solution can be defined as follows.

Definition 2.1. Given an abduction problem as described above, a set $H \subseteq \mathcal{H}$ is a *(standard) abductive solution* for an abduction problem if (if and only if)

- for each $o \in \mathcal{O} : \Sigma \cup H \vdash o$, and
- $\Sigma \cup H \nvdash \perp$,

where $\perp$ denotes the impossible state (*falsum*). Essentially, the first condition says that elements from $\mathcal{O}$ must be derivable from the abductive solution together with background knowledge Σ. The second condition says that Σ and H are consistent.

As an example, consider the following theory Σ about diagnosing a faulty lamp consisting of the Horn clauses:

(1) faulty(L) $\leftarrow$ lamp(L) $\wedge$ current_break(L)
(2) current_break(L) $\leftarrow$ fuse(L, F) $\wedge$ melted_fuse(F)
(3) *lamp*(a)

Let the set of hypotheses be $\mathcal{H} = \{fuse, melted\_fuse\}$. The background theory Σ consists of two rules, (1) and (2), and one fact (3). Suppose we want an explanation for the observation *faulty*(a). Non-creative abduction will not generate a solution since backward-chaining from *faulty*(a) on the rules (1) and (2) produces he set $H' = \{fuse(a, X), melted\_fuse(X)\}$, where the variable X is not instantiated to a constant. Element-creative abduction applies a skolemizing substitution to H', i.e. all variables in H' are uniformly replaced by a new Skolem constant. Informally, a Skolem constant denotes an unknown element of the problem domain. If a skolemizing substitution has to be applied to the abductive solution, it is called *element-creative*. In this case, the abductive solution is $H = \{fuse(a, \alpha), melted\_fuse(\alpha)\}$, where α is a Skolem constant.

O'Rorke et al. [8] describe the key insight in the 'chemical revolution' as an instance of element-creative abduction. The chemical revolution refers to the phase where the phlogiston theory was replaced by the oxygen theory. Given a logical description of the phlogiston theory and the observation that the weight of mercurius calcinatus increases (which contradicts the prediction within the phlogiston theory), element-creative abduction eventually hypothesizes the existence of an unknown component of mercurius calcinatus, which Lavoisier gave the name 'oxygen'. The assumption of the element 'oxygen' eventually led to the formation of a new theory, the oxygen theory.

2.2. Law-creative abduction

The well-known area of *inductive logic programming* (ILP) or *inductive concept learning* [6] can be seen as a form of law-creative abduction, where a *new law* is generated that defines some target concept, such as 'being someone's daughter'. We mention ILP here for its importance as a learning mechanism, although its algorithms considerably differ from those of abduction (see Lavrač and Džeroski [6] for details). In brief, the idea of inductive concept learning with background knowledge is as follows: given a set of training examples $\mathcal{E}$ and background knowledge $\mathcal{B}$ in the form of atomic formulas, find a hypothesis H in the form of a rule, such that all examples that satisfy the concept (the positive examples) are covered by H and no example not satisfying the concept (the negative examples) is covered by H. The hypothesis H defines a target relation $p(X_1,\ldots,X_n)$ in terms of the relations expressed in the background knowledge.

Consider an inductive concept learning problem involving positive and negative examples for the target relation *daughter*(X, Y), and background knowledge expressing *female*(X) and *child*(X, Y) relationships. An inductive solution consists of a rule defining the target relation, such as '$daughter(X, Y) \leftarrow female(X) \wedge child(X, Y)$'.

Observe that both element-creative abduction and ILP explain a set of facts. In the next section, we promote an abduction scheme that may explain a set of *rules*, possibly denoting empirical laws.

3. Creative abduction for scientific discovery

Schurz [15] argues that empirical regularities applying to some (at least one but not all) objects of a domain, called *local temporal regularities* (or simply *empirical* regularities), can be explained by hypothesizing an 'intrinsic property' or 'disposition' of those objects, and calls this form of inference 'abduction to a disposition'. Then he shows that if the regularities are correlated, this form of abduction is able to significantly *unify* a given corpus of knowledge. In this case, the disposition might be called a genuine theoretical term or even a cause. The invention of a disposition effecting more unified knowledge is a basic activity of scientific discovery.

We first define the scheme for disposition-creative abduction. Then we demonstrate the unifying power of this form of abduction, given a set of correlated empirical regularities.

3.1. Inferring dispositions by creative abduction

Assume an abduction problem where the set of observations $\mathbb{O}$ consists of a set of 'condition-effect' rules of the form.[1]

$$\forall t : cxt(a_i, t) \rightarrow e(a_i, t) \quad (1 \leq i \leq n)$$

where t is a (temporal) variable and $a_1,\ldots,a_n$ are constants. It is important to note that n is required to be strictly smaller than the number of all objects in the 'universe of discourse', else those rules can be represented by a single rule, namely '$\forall t \forall x$: $cxt(x, t) \rightarrow e(x, t)$'. The rules in $\mathbb{O}$ denote local temporal regularities, for instance, the object denoted by a_i conducts current (effect e) whenever certain context conditions cxt hold. By contrast to standard abduction problems, no background knowledge is required, i.e. Σ can be empty. Later on, we will assume that Σ contains a set of correlated empirical regularities.

[1] For clarity, we hereafter use more standard logical notation instead of the Prolog-style notation of the previous section.

Definition 3.1. Let a (disposition-creative) abduction problem be given as described above. A pair $\langle H_d, H_r \rangle$ is a *disposition-creative solution* for the abduction problem iff

- H_d is a conjunction of atoms $d(a_1) \wedge \ldots \wedge d(a_n)$, where the predicate d denotes a disposition of a_i $(1 \leq i \leq n)$.
- H_r is a rule of the form
  $\forall x \forall t : d(x) \rightarrow (cxt(x, t) \rightarrow e(x, t))$
- For each $o \in \mathbb{O} : H_r \cup H_d \vdash o$.

Intuitively, we explain a local temporal regularity by the disposition of a_i to bring about some effect e, given context conditions c. Note that the predicate d has no argument position for a temporal argument. Hence we assume that dispositions are either always present or always absent. This is not a limitation of our approach; 'temporary' dispositions can be introduced in the obvious way. Moreover, observe that we are still in the realm of Horn logic since '$\forall x$: $p(x) \rightarrow (q(x) \rightarrow r(x))$' is equivalent to '$\forall x$: $p(x) \wedge q(x) \rightarrow r(x)$'. Actually, Schurz [15] suggests a stronger formula '$\forall x \forall t$: $cxt(x, t) \rightarrow (d(x) \leftrightarrow e(x, t))$' as the invented law. In our discussion, however, we see no need to require that the disposition is identified by the law under consideration.

Since the hypothesized disposition might be seen as a mere *abbreviation* for the observed regularity, we call it a 'first-order' disposition. However, the assumption of a disposition is justified if it explains *multiple correlated* regularities. For instance, we observe that those objects which conduct current when subject to a voltage source, also conduct in hot surroundings (thermal conductivity), and bend under force without breaking (pliability). The correlation of the mentioned regularities can be explained by the 'second-order' disposition of *metallicity*. It is the second-order dispositions which likely correspond to real causes in nature.

As explained below, the merit for KDD lies in the fact that the assumption of second-order dispositions may significantly unify a corpus of knowledge.

3.2. Scientific discovery by knowledge unification

A theory is called *more unified* if more observed events can be explained by a smaller set of laws together with assumed dispositions. To see the unifying power of disposition-creative abduction, assume that for some object a, there exist n different local temporal regularities of the form

$$\forall t : cxt_i(a, t) \rightarrow e_i(a, t) \quad (1 \leq i \leq n)$$

such that all of the n regularities correlate with each other. In effect, we obtain $n \times (n-1)$ rules of the form

$$\forall x \forall t : (cxt_i(x, t) \wedge e_i(x, t)) \rightarrow (cxt_j(x, t) \rightarrow e_j(x, t))$$
$$(1 \leq i \neq j \leq n)$$

Together with the n regularities, we obtain $n \times (n-1) + n = n^2$ rules. On the other hand, disposition-creative abduction generates n rules (laws) of the form $(1 \leq i \leq n)$

$$\forall x \forall t : d(x) \rightarrow (cxt_i(x,t) \rightarrow e_i(x,t))$$

Knowledge unification here corresponds to a reduction from a quadratic to a linear number of rules, where the more unified theory may explain the same number of regularities as the original theory. Even better, if the regularities hold for k objects, we can reduce $n^2 - n + (n \times k)$ rules to n rules.

At this point, let us ask whether disposition-creative abduction meets the criteria for KDD methods. Recall that the obtained knowledge is required to be new, plausible, intelligible, and useful.[2] First, we obtain *new* knowledge in the form of a hypothesized disposition and a corresponding law. Second, the produced knowledge is certainly *plausible* since it allows to unify a given corpus of knowledge. Third, we obtain knowledge that is *intelligible* because it has a concise formulation. Finally, the generated knowledge is *useful* since the invention of second-order dispositions (or causes) provides a more unified view of science, e.g. the assumption of metallicity in chemistry.

The power of disposition-creative abduction as a knowledge discovery method relies on the availability of a large set of correlated empirical regularities (as background knowledge Σ). In general, however, we might not be provided with such expressive background knowledge. In the next section, we introduce a weaker version of disposition-creative abduction that is more broadly applicable to knowledge discovery tasks.

4. Creative abduction for knowledge discovery

We will develop *goal-creative* abduction analogous to disposition-creative abduction. However, goal-creative abduction is weaker in the sense that it assumes 'regularities' of a quite simple and easily available format. As an example, we discuss Web usage mining based on records in a Web server log.

4.1. Inferring goals by creative abduction

As in the case of disposition-creative abduction, we assume that the set of observations $\mathcal{O}$ is given as a set of 'condition-effect' rules that apply to some objects of the domain. However, there is no quantification over time, i.e. the rules have the form

$$cxt(a_i, t_j) \rightarrow e(a_i, t_j) \quad (1 \leq i \leq n, 1 \leq j < \omega)$$

and are called local *transitions* or simply transitions. For instance, if a person sees restaurant X at time point t, the person enters X. At other times, the person might choose a different restaurant. We explain this behavior by the changing *goals* of the person at different times. Here, the term 'goal' is meant as a counter-term to 'disposition' which denotes a permanent property. Instances of 'goal' are 'interest' or 'motivation'. As we already mentioned in the section on disposition-creative abduction, we might also consider dispositions (or goals) that hold in a certain time interval. For simplicity, we take the notion of goal to be momentary, and completely delete the reference to time.

Definition 4.1. Let a goal-creative abduction problem be given analogous to a disposition-creative abduction problem. A pair $\langle H_g, H_r \rangle$ is a *goal-creative solution* for the abduction problem iff

- H_g is a conjunction of atoms $g(a_1) \wedge \ldots \wedge g(a_n)$, where the predicate g denotes a goal of a_i $(1 \leq i \leq n)$.
- H_r is a rule of the form

  $\forall x : g(x) \rightarrow (cxt(x)) \rightarrow e(x))$
- For each $o \in \mathcal{O} : H_r \cup H_g \vdash o$.

Basically, it says that the assumption of a certain goal explains a given transition, and is most probably false since the transition can be triggered by different goals. For instance, there might be many different reasons to enter a restaurant (dining, meeting a friend, looking for lost wallet, and so on). However, as in the case of disposition-creative abduction, the presence of multiple correlated transitions might justify a higher-order goal. Take our restaurant example, and the example of a person entering McDonalds. We might infer that the person likes burgers from McDonalds. Now assume that the same person would choose Mosburger and Burger King as well. Then we can hypothesize the higher-order goal that the person likes any kind of burgers.

In the following, we will first demonstrate how goal-creative abduction in the presence of correlated transitions may unify a given corpus of knowledge, and then discuss a concrete example, namely inferring users' (common) goals based on users' access patterns.

4.2. Knowledge unification by correlated transitions

Assume that for m objects, we are given n transitions of the form

$$cxt_i(a_k) \rightarrow e_i(a_k) \quad (1 \leq i \leq n, 1 \leq k \leq m)$$

which yields $m \times n$ transitions. Furthermore, suppose that for each a_k $(1 \leq k \leq m)$ from a given sample *smpl*, all of the n transitions are correlated, which gives $n \times (n-1)$ rules of the form

$$\forall x : smpl(x) \rightarrow ((cxt_i(x) \wedge e_i(x)) \rightarrow (cxt_j(x) \rightarrow e_j(x)))$$
$$(1 \leq i \neq j \leq n)$$

[2] We acknowledge that it might be difficult to give a precise definition of the feature 'useful'. In the case of 'intelligible', we may use some concepts from information theory, such as the description length of the encoding.

i.e. we obtain $n^2-n+(n\times k)$ rules in total. However, by means of goal-creative abduction and the assumption that the objects $a_1,\ldots,a_m$ are drawn from the sample, i.e. $smpl(a_k)$ for each a_k $(1\leq k\leq m)$, the same set of transitions can be derived from n rules of the form

$$\forall x: g(x)\rightarrow(cxt_i(x)\rightarrow e_i(x))\quad(1\leq i\leq n)$$

which is a significant reduction of the number of rules to encode the given knowledge. Notice that the correlations only hold under the condition that the objects are included in the given sample.

4.3. Web usage mining

Web usage mining is the clustering of Web users based on their browsing activities (Fu et al. [3]). Here users with similar web access patterns can be grouped into classes (or clusters). The identification of such clusters is important, for instance, for the creation of *adaptive Web sites*, where sites automatically improve their organization and presentation based on user access data [11], or in *collaborative recommendation* where sites are recommended to users because other users with similar interests liked the sites [1].

A server access log is a document that contains entries specifying the requests for pages answered by the server. A 'visit' is a sequence of pages accessed by a single user (client) in one period. We take 'period' as the unit of interaction between users and server (e.g. 1 day). Each single request contains at least the client's IP address, the URL requested, and the date/time when the request is received. Hence, a single request, also called *record*, has the form ⟨*user_IP*, *page_URL*, *time*⟩. We assume that records for each user are transformed to *(simple) steps* of the form

$$page(user\_ip_i,page\_url_j)\rightarrow page(user\_ip_i,page\_url_{j+1})$$

$(1\leq i\leq n,\ 1\leq j<m)$, where n is the number of users in a single period, and m is number of pages hosted on the server. Basically, a step tells which link a user activates on a given page. The activated page is uniquely determined by the time entry in the record. Observe that since each step has the format of a transition, goal-creative abduction can be applied to infer the *interest* of a user. However, it seems impossible to identify a user's interest based on a single simple step. If a user is on a toy site and activates a link referring to baby toys, all we can assume is that the user is interested in (has the goal of finding) baby toys. Considering a visit, i.e. a sequence of simple steps, can lead us to further insights about the basic interests of the user. Assume the same user also activates a link referring to baby furniture when on a furniture page, and diapers on the online supermarket site (example borrowed from [3]). Then we can hypothesize that the user has the goal of finding goods related to babies, and may assign her or him to the group (cluster) of 'expecting parents'.

In our example, the *visit-coherence assumption* [11] holds, i.e. the pages a user visits during one visit tend to be conceptually related. On the other hand, a user might have different goals in mind, and might search for baby goods as well as motorcycles. Therefore, we rather consider clusters of groups with similar browsing activities [3], indicating *common and stable interests* of users in the cluster. The set of steps chosen by those users can be readily rewritten in the form of correlated transitions (qualified by the period of interaction *smpl*)

$$\begin{aligned}\forall x: smpl(x)\rightarrow{}&((page(x,page\_url_i)\\&\wedge page(x,page\_url_{i+1}))\rightarrow((page(x,page\_url_j)\\&\rightarrow page(x,page\_url_{j+1})))\end{aligned}$$

such that $1\leq i\neq j<n$. As before, under the assumption that the users are taken from the specified period, we derive the following rules by goal-creative abduction:

$$\begin{aligned}\forall x: g(x)\rightarrow{}&(page(x,page\_url_i)\\&\rightarrow page(x,page\_url_{i+1}))\quad(1\leq i<n)\end{aligned}$$

In the 'baby' example, the abduced goal might express the interest in all kinds of baby goods, indicating that the user belongs to the group of expecting parents. This information can be used to recommend links relevant to baby goods, if the user is observed to be interesting in, e.g. baby toys, or to create an index page.

5. Discussion

We presented two forms of creative abduction that are intended to cover different enterprises within KDD. The first one is called *disposition-creative abduction* and can be applied to the task of theory formation in scientific discovery. Disposition-creative abduction is closely related to Reichenbach's principle of the *common cause* [14], i.e. whenever two events A and B are correlated statistically (or deterministic), then they must have a (temporally prior) common cause. The assumption of common causes can also be compared to the invention of 'hidden variables' in Bayesian networks [4,9]. In a situation where there exist mutual dependencies among variables, it is suggested to invent *hidden variables* that explain the dependencies and render the variables conditionally independent. Those variables are called 'hidden' since, similar to causes or dispositions, they are not directly observable. However, significant differences exist between the assumption of dispositions and the invention of hidden variables. We can only deal with deterministic relationships, whereas the Bayesian network approach is probabilistic in nature. On the other hand, our approach is intrinsically first-order, whereas Bayesian networks are propositional. Hence, we are able to formulate more compact (new) laws or theories.

The second form of creative abduction, *goal-creative* abduction, is weaker since it is based on local transitions instead of empirical regularities. Here the unifying power of (goal-)creative abduction can be effected by the presence of correlated simple 'condition-effect' rules, such as single steps in the browsing activity of a Web user. Web usage mining by means of goal-creative abduction is intended to infer basic interests of a group of Web users by comparing their server access patterns. For a single user, Sunayama et al. [16] infer the user's basic interests from search queries put to a search engine, similar to the invention of hidden variables in Bayesian networks. From a user modeling point of view, their approach and our approach are complementary in the sense that they base the inference to the users' interests on the co-occurrence of events (search words), while our approach is based on page-to-page transition steps.

6. Conclusion

In this paper, we advance creative abduction as a unifying framework for knowledge discovery. Variants of creative abduction subsume important discovery tasks such as theory formation and revision, data mining, and inductive concept learning. In particular, we focus on a form of creative abduction where a disposition or goal is hypothesized in order to explain observed regularities: disposition-creative and goal-creative abduction. Both of them produce knowledge that is new, plausible, intelligible, and useful. The knowledge obtained by disposition-creative abduction is more plausible than that of goal-creative abduction, since the former is based on stronger background knowledge, namely local temporal (empirical) regularities. On the other hand, goal-creative abduction seems more useful than the disposition-creative version, because it assumes only weak background knowledge in the form of so-called 'transitions'. As an example of a transition we discussed a simple Web browsing step. However, following our aim to focus on underlying theory rather than systems, the application of goal-creative abduction to Web data mining is shown only conceptually. Future work will include empirical studies and comparisons with other approaches.

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