THE INTERDEPENDENCIES OF THEORY FORMATION, REVISION, AND EXPERIMENTATION

by

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June 1988

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SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION: Unclassified	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT: Approved for public release; distribution unlimited
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S): UIUCDCS-R-88-1439	5. MONITORING ORGANIZATION REPORT NUMBER(S)
6a. NAME OF PERFORMING ORGANIZATION: University of Illinois Dept. of Computer Science; 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION: Cognitive Science (Code 1142CS) Office of Naval Research
6c. ADDRESS (City, State, and ZIP Code): Urbana, IL 61801	7b. ADDRESS (City, State, and ZIP Code): 800 North Quincy Street Arlington, VA 22217-5000
8a. NAME OF FUNDING/SPONSORING ORGANIZATION; 8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER: N00014-85-K-0559
8c. ADDRESS (City, State, and ZIP Code)	10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO.
61153N	RR04206	RR04206-0A	NR667-551

11. TITLE (Include Security Classification)

The Interdependencies of Theory Formation, Revision, and Experimentation (Unclassified)

12. PERSONAL AUTHOR(S)

Brian Falkenhainer and Shankar Rajamoney

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Technical Report	FROM 85-9-1 TO 88-8-30	88-6-1	14

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	
05	08		

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This paper depicts theory development as a synergistic cooperation of scientific methodologies, each focusing on different aspects of the problem. It discusses how they may be integrated to provide a more unified and comprehensive treatment of scientific theory discovery. ~~We describe~~ a general protocol is described for interaction between theory formation, theory revision, and experimentation. This protocol enables theory formation to make specific queries about the state of the world to fulfill its hypothesis generation goals. It also enables epxerimentation-based revision to post tasks for theory formation to supply relevant hypotheses. The utility and generality of this protocol is demonstrated by an implementation which integrates two previously autonomous systems. Its performance is described for discovering and revising models of evaporation and osmosis.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT: ☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	21. ABSTRACT SECURITY CLASSIFICATION: Unclassified	
22a. NAME OF RESPONSIBLE INDIVIDUAL: Dr. Susan Chipman	22b. TELEPHONE (Include Area Code): 202-696-4318	22c. OFFICE SYMBOL: ONR 1142 PT

DD Form 1473, JUN 86 — Previous editions are obsolete. — SECURITY CLASSIFICATION OF THIS PAGE

REPORT NO. UIUCDCS-R-88-1439

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Supported in part by an IBM Graduate Fellowship to Falkenhainer, by a University of Illinois Cognitive Science / Artificial Intelligence Fellowship to Rajamoney, and by the Office of Naval Research under grants N00014-85-K-0559 and N00014-86-K-0309.

1. Introduction

Scientific discovery follows a cyclic pattern of theory development – the formation of a new theory, a number of fixes to account for anomalous behavior and, later, when the fixes result in a grossly inelegant theory, a paradigm shift that radically transforms the old theory (Kuhn, 1970). Theory development is a multi-faceted process involving the synergistic cooperation of a number of approaches. This paper attempts to provide a comprehensive model for each stage of theory development by integrating several techniques – empirical learning, analogical learning, and experimentation.

Our central task is to provide causal explanations of observed natural phenomena, using an imperfect or non-existent theory of the domain. This paper describes the integration of two techniques: *verification-based analogical learning*, which is used primarily for theory formation (including paradigm shifts), and *experimentation-based theory revision*, which is used primarily for theory testing and revision. (We review each only briefly here, for details see (Falkenhainer, 1987) and (Rajamoney, 1988)). Analogy-driven theory formation can develop novel theories in a focused manner, drawing from its knowledge of analogous precedents. However, in isolation it lacks the ability to examine the state of the world and experimentally confirm or refute hypotheses. Experimentation-based theory revision, on the other hand, is well suited to modifying theories and testing the different modifications to a theory. However, it has very little guidance during the task of proposing different modifications to a theory. Also, it must rely on fortuitous observations or prediction failures to initiate theory revision.

In this paper, we describe a set of general principles underlying theory formation, theory revision, and experimentation. We demonstrate how these techniques, each focusing on different aspects of the problem, may be integrated to provide a more unified and comprehensive treatment of scientific theory development. In particular, we show how experimentation is used to empirically guide and verify the analogy-driven theory formation stage and how analogy is used to initiate and focus the experimentation-based theory revision stage. Furthermore, we outline a general protocol for communication between theory formation and experimentation-based revision which solves many of their individual problems. Experimental queries using the protocol are motivated by empirical questions and requirements encountered during hypothesis generation and evaluation. Theoretical queries are motivated by the need for plausible hypotheses during experimentation-based theory revision.

The utility and generality of this protocol is demonstrated by an implementation integrating two previously autonomous systems: PHINEAS, which performs verification-based analogical learning, and ADEPT, which performs experimentation-based theory revision. When confronted with a novel observation of evaporation, this integrated architecture and its associated protocol enabled PHINEAS to empirically question the necessity of heat flow (e.g., from a stove) in its evaporation hypothesis derived from boiling. In turn, the protocol enabled ADEPT to be advised of vapor saturation as a candidate explanation for why evaporation stopped.

We conclude this section with a review of the two techniques. An integrated design and the general principles which emerge is then described in section 2 and made concrete with the use of an implemented example. An additional example is briefly provided in section 3.

1.1. Verification–Based Analogical Learning: An Overview

Verification–based analogical learning (VBAL) (Falkenhainer, 1987) is an approach to theory formation and revision which relies on analogical inference to hypothesize new theories, and *gedanken* experiments (i.e., simulation) to analyze their validity. VBAL is an iterative process consisting of four primary stages:

1. **Behavior match.** An anomalous observation triggers a search for previously understood experiences that exhibited analogous behavior. The result of this stage is a candidate analogue and an initial set of correspondences between the two domains.[1]
2. **Theory generation.** The central objective of the second stage is to produce a fully operational initial hypothesis about the current domain. This stage has two components. First, the model used to explain the recalled experience is analogically mapped into the current domain. This mapping is guided by the initial correspondences found in the behavioral comparison. Second, the model must be *operationalized* if it is not already. For example, it may reference entities and properties that are currently unknown. These entities and properties must either be inferred from the domain theory or their existence must be postulated.
3. **Theory completion.** The operational model may not necessarily conform to the present observation. Thus, theory revision may be required to examine predictions and produce a consistent initial model. Revision in VBAL is based on passive consistency – when empirical experiments are impossible, prefer minimal revisions with an analogical precedent.
4. **Theory revision.** While the current domain model may accurately account for all known observations, a new situation may be observed for which the model is inadequate.

PHINEAS, the current implementation of VBAL, uses Forbus' (1984, 1986) *Qualitative Process theory* to represent and reason about change in the physical world, and a modified version of Gentner's (1983) *Structure-Mapping theory* for analogical mapping. The system's primary analogy component, SME (Falkenhainer et al, 1986), is used to perform comparisons of similarity and map theories across domains. PHINEAS has been shown to discover a caloric theory of heat by analogy to liquid flow. It has also developed an explanation of oscillatory electrical circuits from its knowledge of mechanical oscillation.

1.2. Experimentation–Based Theory Revision: An Overview

Experimentation–based theory revision (Rajamoney, 1988) is an approach to changing or augmenting an incomplete or incorrect theory. Experimentation–based theory revision consists of three main steps:

1. **Contradiction detection.** Problems with the existing theory are detected by comparing the predictions based on the theory with the observations made from the real world. If the predictions and observations lead to a *contradiction* then the existing domain theory has to be revised.

[1] The term *analogue* is used in its most general sense throughout this paper. An analogy may be found within the same domain, as between one instance of liquid flow and another, or across domains, as between electron flow and liquid flow. No strong claims are made about the access mechanism, whose theoretical underpinnings are still under development. While implemented and autonomous, the accesser is far from sophisticated at this time.

2. **Hypothesis formation.** Hypotheses that involve changes to the existing theory are proposed. This stage is governed by *explanation construction* – only changes leading to a revised domain theory that can explain the observed phenomenon are proposed.
3. **Experiment design.** Typically, there will be a number of different ways to change a theory to explain a new phenomenon. Experiments are designed to identify the change that is consistent with the actual behavior of the real world (see Rajamoney, 1988). Hypotheses whose predictions are not consistent with experimental observations are rejected.

ADEPT is a system that demonstrates experimentation-based theory revision. It starts with an operational but initially incomplete and incorrect theory and revises it to conform to observations made from the real world. ADEPT has been demonstrated on a number of examples. It has successfully learned effects and conditions of physical processes such as a new influence of evaporation on the temperature of the evaporating liquid and a new condition for dissolving solutes requiring the concentration of the solution to be less than its saturation concentration.

2. An Integrated Model of Theory Development

Theory development is a dynamic process involving the formation of candidate theories, revisions to account for anomalous observations or achieve simplicity, and experimentation to test hypotheses and collect new data. These activities are highly interdependent yet highly modular. They may be performed by numerous people in distant locations, possibly across generations (e.g., the discourse between Copernicus, Galileo and Kepler, whose lives spanned nearly 200 years). In this section we develop this "collection of specialized experts" view of theory development with respect to theory formation, revision, and experimentation and show how the expertise of each is required to reduce the search space throughout the development cycle. We first describe strengths and limitations of our two methodologies and their complementary relationship. We then define a general protocol for interaction between systems specializing in theory formation, revision, and experimentation. Next, we show how the integrated system provides a comprehensive model for each stage of theory development.

2.1. Limitations and Strengths

As independent research efforts, each approach is designed to perform theory development autonomously. VBAL conjectures explanations of the new behavior based on its similarity to previously encountered phenomena. Its power lies in its ability to construct novel theories, focused by considering only theories for which it has an analogical precedent. However, VBAL has some important limitations. It is intended for passive observation and thus does not empirically test a hypothesis. It makes intermediate assumptions and depends on simulation experiments to test the consistency of these assumptions. This leads to questions about the validity of proposed theories. In addition, VBAL must rely on heuristics and prior experiences to guide search, thus requiring one to entertain hypotheses that might easily be empirically refuted.

In turn, experimentation-based theory revision locates known theories that appear relevant to the observation and modifies them to inclusively account for the new example. Its power lies in its ability to interact actively with the world, discriminate among alternative revisions, and refute proposed hypotheses. However, experimentation-based theory revision has some important limitations. It is unable to make large, fundamental modifications to a theory, or produce one where none existed before. This limits it to revising "roughly correct" theories. Furthermore, experimentation is essentially open-ended in terms of what tests can be made and what kinds of experiments can be designed. For example, it may not be tractable to collect all possible hypotheses prior to conducting experiments.

The limitations of each approach corresponds nicely to the strengths of the other. Verification-based analogical learning provides:

1. Highly focused, theoretically motivated queries about the state of the world, such as checking for the existence of an anticipated object or testing theoretical predictions.
2. Large changes in theoretical perspective, develops new theories and provides candidate theories to revise.
3. A restricted number of potential hypotheses and a preferential ordering on hypotheses.

Experimentation-based theory revision provides:

1. Empirical tests for the relevance of certain perceived aspects of a situation, such as the necessity of ancillary processes normally associated with an analogue theory.
2. Discrimination among plausible hypotheses or refutation of a single hypothesis.
3. Experiments to detect the presence of an unnoticed or conjectured object or tests for conjectured properties of existing objects.
4. Probes of the situation for unknown values of a quantity or its derivatives.

2.2. A Communication Protocol

In this section we develop a general protocol for theory development tasks which enables one method to make use of another's expertise in a system independent manner. If the process answering a query lacks the appropriate decision procedure or is unable to successfully produce a response, a value of `UNKNOWN` is always acceptable. The protocol results in an extendible architecture, allowing new techniques to be added or existing techniques to be replaced by improved versions.

A crucial question concerns how one tells whether or not some fact holds. In theory formation and revision, we must assume incomplete knowledge. Thus, normal ways of deriving facts about the environment must be redefined. We distinguish between queries which depend primarily on the current beliefs of the system and queries which are able to question those beliefs by looking for alternate sources of information. *Direct queries* directly probe for the status of a condition using inference, or simple empirical tests if their status is not easily deducible. *Indirect queries* look for the effects normally associated with a condition, to test if deductive conclusions are wrong or if an analogous condition is in effect.

We decompose theory development into eight tasks, which suffice for a wide range of interesting problems:

Present? <object-or-variable> <primary-conditions> <secondary-conditions>
This queries for the existence of a partially specified, unknown object. Failure of any secondary conditions is not grounds for rejection, but may be used to reduce the set of candidates satisfying primary conditions. For example, investigation of a chemical reaction

may lead one to suspect and test for the presence of a particular catalyst in the mixture.

Test–Value <quantity> <value>
This instructs the system to search for an inferential determination of the quantity's value, or experimentally probe the situation for the value. The value may be left unspecified, or the truth of a particular relative value may be sought, as in `(GREATER-THAN boiling-temperature)` or `DECREASING`. For example, hypothesis generation may require the value of a quantity not reported in the initial observation.

Test–Condition <relation>
This determines if the specified relation holds. For example, investigation of heat-related theories may require determining if one object is in thermal contact with another.

Test–Effects <relation>
This is an indirect query which instructs the experimentation system to look for the presence of the known effects of a physical relation. For example, if `Test-Condition` had determined that a specified fluid path was not configured to support liquid flow, the validity of this conclusion may be questioned by looking for the effects of liquid flow through the path. `Test-Effects` may be used to seek an answer when `Test-Condition` returns unknown, instigate belief revision, or create a new concept analogous to the given physical relation.

Necessary? <condition> <observation>
The necessity of a condition thought to be essential to achieving an observation is questioned with this query. For example, a developing theory on chemical reactions may state that a particular catalyst is required. This query would call for experiments to determine if the catalyst is actually required.

Discriminate <hypotheses> <observation>
This asks the experiment design system to construct experiments to discriminate among a set of hypotheses that are thought to cause the observation. For example, during theory revision, several modifications of the original theory may explain the novel observation. This query finds those revisions that are consistent with information gathered from directed experiments.

Propose–Theories <observation>
This invokes the theory formation system to develop theories that will explain the observation. For example, during theory revision, experiments may rule out all the candidate revisions or the revision proposer may not find any consistent modifications to the theory. In such cases, the theory revision system uses this query to post a theory formation task.

Propose–Revisions <observation> <theory> <:condition or :effect>
This query asks the theory formation system, or a specialist in revision hypotheses, to propose revisions to a theory that will enable it to explain the observation. The query must specify if the revision should be to the theory's conditioning relations or to its set of effects.

2.3. The Three Stages to Developing a Complete and Consistent Theory

There are three primary stages to theory development within the VBAL framework: *Theory Generation*, *Theory Completion*, and *Theory Revision*. This section examines the interaction of the two systems in each of these stages and uses an implemented example to illustrate the interaction. The example involves forming and revising a model for *evaporation*. Throughout this section, we will assume that theories are represented by a set of *processes* and *individuals* (objects) as defined in Forbus' (1984) Qualitative Process theory. Each process specifies a set of participatory *individuals* (objects and othei processes), a set of *conditioning relations* indicating when it is active, and a set of *effects* that apply when it is active.

In our implementation of this integrated architecture, PHINEAS initiates the process of explaining new observations and posts tasks for ADEPT when its expertise is required. If an observation cannot be explained by existing theories, PHINEAS attempts to generate an explanation by recalling past observations of similar or analogous behavior. The knowledge used to explain these previous observations is used to analogously explain the current situation. In constructing the explanation, PHINEAS may call on ADEPT to measure the value of a quantity or determine the existence of a hypothesized object. In addition, experimentation and possible revision of the initial hypothesis may then be required for this or future observations. PHINEAS and ADEPT use the protocol to interactively solve such problems during theory formation and revision.

2.3.1. Theory Generation

Theory generation is the process of proposing an initial theory to explain a novel phenomenon. There are two stages to theory generation in VBAL. The first stage examines the current behavior and recalls previously understood similar behavior. Theories used to explain an analogue behavior are then mapped into the current domain and proposed as an initial explanation of the current phenomenon.

The system next divides the elements of each hypothesized theory into *primary processes* and *ancillary processes.* A primary process is one that affects an observed quantity, such as the temperature of an object whose temperature was observed. Ancillary processes are those that were used in explaining the analogue case, but do not directly affect one of the current observables. The necessity of a primary process is assumed and never experimentally questioned. Ancillary processes are eliminated during theory formation if they are found to be unnecessary.

The second stage in theory generation is to make the proposed explanations operational. A model is non-operational if it calls for participatory objects and processes whose presence was not noticed during the initial observation. If their existence cannot be determined (at this time), their existence must be assumed or the proposal modified to not depend on them. Operationalization first consists of instantiating each primary process by examining its unknown individuals:

When the individual is an uninstantiated, ancillary process:
  Attempt to instantiate it.
  If not instantiable, test for `NECESSARY?`.
    If necessary, reclassify it as a primary process, otherwise remove it.
When the unknown individual is an entity:
  Test for `PRESENT?`
  If not, postulate its existence and store its known set of characteristics.

Any ancillary process that is experimentally determined to be irrelevant is deleted from the generated theory. Remaining ancillary processes must be instantiated, if they have not been already. However, if that instantiation calls for postulating the existence of an unknown entity, (Necessary? <ancillary-process> <observation>) will be invoked first. If a later contradiction occurs, the ancillary processes should be the first to be questioned during revision.

The final step in producing a fully operational theory is to test the analogically proposed conditioning relations for validity under the current conditions. This is done using `Test-Value` and `Test-Condition`. Conditioning relations not known to be true in the current context are temporarily removed in order to obtain a fully operational theory and enable discrimination with competing theories. For surviving theories, an attempt is then made to replace these conditioning relations with analogous relations applicable to the current context.

2.3.1.1. Evaporation Example: Generating Initial Hypotheses

This section describes how the integrated implementation generates an initial model for evaporation. The system begins with knowledge of six processes - liquid flow, heat flow, dissolving, spring oscillation, boiling and heat replenishment (to constantly maintain the heat of a stove). It also has a database of physical observations fully explained by these processes. Suppose an open beaker containing alcohol is left on a table top for a day, during which time the amount of alcohol is observed to decrease. The problem is to propose an explanation for this observation, which, according to the system's existing knowledge, should never have happened.

Model Creation: At this point, no known, instantiable theory is able to even partially explain the loss of alcohol in the beaker. By examining its knowledge of "similar" behaviors, PHINEAS determines that the only known examples of a liquid leaving a container call for it to flow out or to boil away. Three ordered, initial hypotheses, based on overall behavioral similarity, are generated. The first calls for the alcohol to flow out, the second calls for it to vaporize, and a distant third calls for it to dissolve based on its gradual disappearance. The initial vaporization explanation is shown in Figure 1. It consists of one primary process - boiling, and two ancillary processes - heat flow and heat replenishment, which are believed to be required for boiling to take place.

Model Operationalization: The three models (based on flow, boiling, and dissolving) call for the presence of objects that were undetected in the initial observation. We focus first on operationalizing the vaporization explanation. This explanation requires the presence of two unknowns - alcohol vapor in the beaker and a heat source. PHINEAS first produces the query:

```
(Present?  ?STEAM1  ((Contained-Gas ?STEAM1)          ;primary conditions
                     (Container-of ?STEAM1 beaker)
                     (Substance-of ?STEAM1 alcohol))
                    ())                               ;no secondary conditions
```

Notice that the query is very specific - the object is fully specified and all that remains is to test if it is there. Of course, even this test can be non-trivial. To answer the query, ADEPT first examines the known set of objects and finds that none satisfy the primary conditions. It then examines its database of experimentation techniques, and recalls that litmus paper changes color in the presence of alcohol and can be used to test for the hypothesized presence of alcohol vapor in the beaker. The litmus paper test is conducted, via instructions to the assumed human assistant (such as, "make the litmus paper touch the air inside the beaker"), and a positive result confirming the presence of alcohol vapor is obtained.

```
ACCESS: Found the following applicable to observation OBSERVATION-1
  BMAP(2-CONTAINER-LF,OBSERVATION-1)
  BMAP(BOILING-PROTOTYPE,OBSERVATION-1)
  BMAP(SALT-DISSOLVING,OBSERVATION-1)
 . . .
(B-EXPLAINS
 (SET (PROCESS-DEFINITION PI1        ;derived from heat flow. An ancillary process.
       (IMPLIES
        (AND (INDIVIDUAL ?STOVE (CONDITIONS (QUANTITY (HEAT ?STOVE))))
             (INDIVIDUAL ALCOHOL1 (CONDITIONS (QUANTITY (HEAT ALCOHOL1))))
             (INDIVIDUAL BEAKER1 (CONDITIONS (HEAT-PATH BEAKER1)
                                             (HEAT-CONNECTION BEAKER1 ?STOVE ALCOHOL1)))
             (HEAT-ALIGNED BEAKER1)
             (GREATER-THAN (A (TEMPERATURE ?STOVE)) (A (TEMPERATURE ALCOHOL1))))
        (AND (QUANTITY (HEAT-FLOW-RATE PI1))
             (Q= (HEAT-FLOW-RATE PI1) (- (TEMPERATURE ?STOVE) (TEMPERATURE ALCOHOL1)))
             (I+ (HEAT ALCOHOL1) (A (HEAT-FLOW-RATE PI1)))
             (I- (HEAT ?STOVE) (A (HEAT-FLOW-RATE PI1))))))
      (PROCESS-DEFINITION PI2        ;derived from boiling. The primary process.
       (IMPLIES
        (AND (INDIVIDUAL ALCOHOL (CONDITIONS (SUBSTANCE ALCOHOL)))
             (INDIVIDUAL BEAKER1 (CONDITIONS (CAN-CONTAIN BEAKER1 ALCOHOL)))
             (INDIVIDUAL ALCOHOL1 (CONDITIONS (CONTAINED-LIQUID ALCOHOL1)
                                              (CONTAINER-OF ALCOHOL1 BEAKER1)
                                              (SUBSTANCE-OF ALCOHOL1 ALCHOHOL)))
             (INDIVIDUAL ?STEAM1 (CONDITIONS (CONTAINED-GAS ?STEAM1)
                                             (CONTAINER-OF ?STEAM1 BEAKER1)
                                             (SUBSTANCE-OF ?STEAM1 ALCHOHOL)))
             (INDIVIDUAL PI1 (CONDITIONS (PROCESS-INSTANCE HEAT-FLOW PI1)
                                         (DESTINATION PI1 ALCOHOL1)))
             (ACTIVE PI1)
             (NOT (LESS-THAN (A (TEMPERATURE ALCOHOL1)) (A (TBOIL ALCOHOL1))))
             (GREATER-THAN (A (AMOUNT-OF ALCOHOL1)) ZERO))
        (AND (QUANTITY (VAPORIZATION-RATE PI2))
             (Q= (VAPORIZATION-RATE PI2) (HEAT-FLOW-RATE PI1))
             (GREATER-THAN (A (VAPORIZATION-RATE PI2)) ZERO)
             (I- (HEAT ALCOHOL1) (A (VAPORIZATION-RATE PI2)))
             (I- (AMOUNT-OF ALCOHOL1) (A (VAPORIZATION-RATE PI2)))
             (I+ (AMOUNT-OF ?STEAM1)) (A (VAPORIZATION-RATE PI2)))))
      (PROCESS-DEFINITION PI3        ;derived from heat replenishment. An ancillary process.
       (IMPLIES
        (AND (INDIVIDUAL ?STOVE (CONDITIONS (HEAT-SOURCE ?STOVE)))
             (INDIVIDUAL PI1 (CONDITIONS (PROCESS-INSTANCE HEAT-FLOW PI1) (SOURCE PI1 ?STOVE)))
             (ACTIVE PI1))
        (AND (EQUAL-TO (D (HEAT ?STOVE)) ZERO)
             (I+ (HEAT ?STOVE) (A (HEAT-FLOW-RATE PI1)))))))
  OBSERVATION-1)
```

Figure 1: Creating an initial explanation of the evaporation observation. Here, PHINEAS hypothesizes, via behavioral analogy, that the set of three boiling-related processes explains the evaporation observation. At this stage, these processes are non-operational.

PHINEAS next produces a `Present?` query for the heat source. In this case, ADEPT returns a value of unknown: unable to deductively locate such an object or experimentally test for one. PHINEAS responds with

```
(Necessary? PI1 OBSERVATION-1)
```

which asks if the ancillary process PI1 (heat flow) is necessary to produce the observation. ADEPT proposes to repeat the observation, only this time thermally isolating the alcohol from potential heat flows by using an insulated container. When the amount of alcohol still decreases, the need for an external supply of heat is removed since it must be irrelevant to a potential explanation.

At this point, the vaporization explanation is fully instantiated and consists of a single, vaporization process. To make it fully operational, PHINEAS concludes with the following two queries about its proposed conditioning relations:

```
(Test-Value  (A (Temperature alcohol1))  ¬(Less-Than (A (TBoil alcohol1))))
(Test-Value (A (Amount-of alcohol1)) (Greater-Than zero))
```

ADEPT determines that the first condition is false and the second is true. PHINEAS then deletes the first condition and retains the second condition in the vaporization model.[2] At this stage, the newly-formed vaporization model is completely instantiated, operational, and can fully explain the observed decrease in the amount of alcohol in the beaker.

The experimentally determined answers to these theoretically-motivated questions enabled the system to (1) confirm that alcohol vapor is present, (2) find that no known heat source exists, (3) determine that the type of heat flow associated with boiling is not a necessary component of the newly generated model of evaporation and (4) find that the boiling temperature is not required for the new process. A new *evaporation* model is conjectured as the explanation. The alternative derived from liquid flow is rejected due to the need to hypothesize the existence of unobservable entities (e.g., a destination liquid), which was not required of the evaporation model (i.e., Occam's razor).[3]

2.3.2. Theory Completion

Once an operational model has been produced, it must be tested for consistency with the observed behavior by using it to *envision* (Forbus, 1984) the possible behaviors of the current physical configuration. This corresponds to asking the question "what are the consequences of assuming this new theory?" Simulation may produce unanticipated theoretical predictions or uncover unanticipated interactions with existing theories (Falkenhainer, 1987). Experimentally testing theoretical predictions enables the system to refute a given hypothesis or strengthen its credibility. When unanticipated interactions among theories nullify the anticipated consequences of a hypothesized model, these interactions must be analyzed and theories revised.

At the close of theory completion, a (potentially empty) set of hypothesized models exists that completely and consistently explain the observed behavior. If more than one hypothesis is produced, the `DISCRIMINATE` task is used to eliminate those that can be experimentally refuted.

[2] At model selection time, the attempt to restore the temperature condition fails when no analogous condition can be found.

[3] Once the need arose to hypothesize unseen entities, PHINEAS's agenda mechanism temporarily abandoned the liquid flow approach in favor of the boiling approach. The success of the boiling approach caused the system to permanently abandon the partially complete liquid flow hypothesis. Being third in preference, the dissolving hypothesis was never examined.

2.3.2.1. Evaporation Example: Completing the Theory Formation Process

The operational vaporization hypothesis contains the following three influences:

```
(I- (Heat alcohol1) (A (Vaporization-Rate PI2)))
(I- (Amount-of alcohol1) (A (Vaporization-Rate PI2)))
(I+ (Amount-of alcohol-vapor1) (A (Vaporization-Rate PI2)))
```

The influences on amount are consistent with the initial observation that the amount of alcohol liquid decreased. However, when this model is used to anticipate what will happen to a beaker of alcohol left sitting on a table, it produces two secondary predictions – the alcohol's temperature will drop, due to the loss of latent heat during vaporization, and the amount of vapor will increase. Since the alcohol's temperature across time was not originally reported, `Test-Value` is invoked for the anticipated change in temperature. ADEPT calls for the physical scenario to be repeated and changes in alcohol temperature noted. This test confirms the evaporation theory's hypothesis and verifies it as a complete and consistent explanation for the observed phenomenon.

2.3.3. Theory Revision

Theory revision occurs when an anomalous observation violates an existing model. The first step to revising an imperfect theory is blame assignment, which is done in a layered manner. First, hypotheses are made to determine if the contradiction is due to a process being incorrectly active or inactive, or if a process has an inappropriate causal effect. Once candidate processes have been identified, specific revision hypotheses are generated to modify either the process' conditions or its causal effects. Experimentation is used at each stage to eliminate refutable hypotheses. Experiments are proposed until the correct revision to the theory is found or until all hypotheses have been eliminated. This last case calls for a new round of theory formation.

2.3.3.1. Evaporation Example: Accounting for New Anomalous Observations

The newly formed theory of evaporation predicts that it will always be active as long as there is liquid in a container. When this theory is used to explain a second example of evaporation – evaporation in a closed container – a contradiction is detected when the amount of liquid stops decreasing after only a little liquid has disappeared. Since the system recognizes this as an instance of evaporation (which stopped too soon), ADEPT is invoked to revise the current model. It first determines experimentally that the problem is due to a failed conditioning relation rather than a failed effect relation. It thus queries PHINEAS (using `PROPOSE-REVISIONS`) for a set of candidate conditioning revisions. PHINEAS again recalls liquid flow and dissolving, due to their behavioral similarity and on the grounds that they were both observed to stop after being active for some time (i.e., the relevant problem with evaporation). Through analogous explanations for stopping, it proposes two new candidate quantity conditions – the amount of liquid has to be greater than the amount of vapor (from liquid flow) or the amount of vapor has to be less than some saturation point for the vapor (from dissolving). ADEPT experimentally refutes the first (by constructing an experiment to increase the amount of liquid and observing that evaporation does not start again) and finds the second to be consistent with experiments. This new saturation quantity condition is added to the evaporation model, yielding a theory consistent with existing experiences (Figure 2).

```
(PROCESS-3318
      Individuals  ((?V-3309 (Substance ?V-3309))
                    (?V-3310 (Can-Contain ?V-3310 ?V-3309))
                    (?V-3311 (Contained-Liquid ?V-3311)
                             (Container-of ?V-3311 ?V-3310)
                             (Substance-of ?V-3311 ?V-3309))
                    (?V-3312 (Contained-Gas ?V-3312)
                             (Container-of ?V-3312 ?V-3310)
                             (Substance-of ?V-3312 ?V-3309)))
      QuantityConditions  ((Greater-Than (A (Amount-of ?V-3311)) zero)
                           (Less-Than (A (Amount-of ?V-3312)) (A (Saturation-3326 ?V-3312))))
      Relations  ((Quantity (Vaporization-Rate ?self))
                  (Greater-Than (A (Vaporization-Rate ?self)) zero))
      Influences ((I- (Heat ?V-3311) (A (Vaporization-Rate ?self)))
                  (I- (Amount-of ?V-3311) (A (Vaporization-Rate ?self)))
                  (I+ (Amount-of ?V-3312) (A (Vaporization-Rate ?self)))))
```

Figure 2: The hypothesized model of evaporation in its final, revised form.

3. An Additional Example: Understanding Osmosis

Consider a case of forming and revising a model for *osmosis*. In this example, the system is shown two containers separated by a partition which, unknown to the system, is semi-permeable (Figure 3). It observes the amount of solution decreasing in one container and increasing in the other. The system is unable to explain these observations since none of the known processes are active. A number of processes are candidates for revision: absorption, boiling, condensation, evaporation, or flow. However, due to its ability to detect behavioral similarity, the system focuses first on liquid flow. Using the `Present?` query, it finds two potential paths for a flow: the membrane separating the two solutions and the wall of their shared container. PHINEAS then finds, using `Test-Condition`, that neither object is `Fluid-Aligned` (able to transport fluids), since they are solid objects. It temporarily removes this precondition to form two operational, competing theories. ADEPT, in response to a `Discriminate` task, experimentally rules out flow through the container wall while all experiments continue to substantiate the membrane hypothesis. Now that it has a complete and consistent theory, PHINEAS looks for an analogue to the `Fluid-Aligned` precondition. After positively testing for the effects of the more general *aligned* concept, PHINEAS hypothesizes an analogue to `Fluid-Aligned` (called `Aligned-3417`), which ADEPT determines is a function of the membrane substance. The dependency of osmosis on concentration may then be determined during revision to accommodate future observations (as in Rajamoney, 1986).

4. Evidence from the History of Science and Psychology

History is filled with examples of analogy being used for hypothesis generation. followed by systematic analysis and experimentation (e.g., Oppenheimer, 1956; Dreistadt, 1968; Gentner & Jeziorski, 1987). For example, Black's theories of latent heats of vaporization were developed by analogy with previously theories of melting. A year later, when a steady heat source was available, he conducted quantitative experiments (Roller, 1961). One particularly clear example

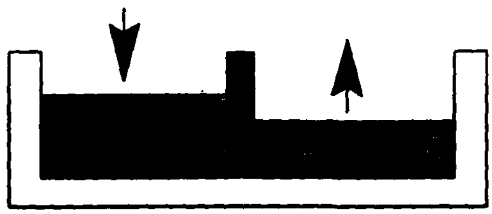

Figure 3: Osmosis example. The solution level in the left chamber is decreasing, while the solution in the right chamber is increasing.

of analogical hypothesis generation appears in Carnot's use of an elaborate analogy between water–driven and heat–driven engines in his development of the Carnot cycle:

> In the waterfall the motive power is exactly proportional to the difference of level between the higher and lower reservoirs. In the fall of caloric the motive power undoubtedly increases with the difference of temperature between the warm and the cold bodies; but we do not know whether it is proportional to this difference... It is a question which we propose to examine hereafter. (Carnot, 1977, page 15)

This hypothesis was later experimentally verified and may now be derived from the first law of thermodynamics. While Carnot assumed the caloric theory, the Carnot cycle and Carnot principle laid the foundations for the second law of thermodynamics, which is independent of caloric or mechanical theories of heat. The psychological literature also includes numerous studies of people using analogy to hypothesize solutions to problems or explanations of physical behavior. Construction of mental or physical experiments is a commonly observed post-hypothesis behavior (e.g., Clement, 1986; Collins & Gentner, 1987).

5. Related Work

Unlike the data–driven, weak methods of traditional systems in machine discovery such as BACON, STAHL, DALTON (Langley et al, 1981, 1987) and ABACUS (Falkenhainer et al, 1986), our system is theory–driven and knowledge–intensive. More closely related to our integrated model of theory formation, revision, and experimentation are Dietterich and Buchanan's (1983) EG and Shrager's (1987) IE. EG stressed the need for experimentation in theory formation and focused on how experimentation could constrain a potentially unwieldy hypothesis generator. While we incorporate this aspect, we also emphasize the important role that a highly focused theory generator may have on experimentation. In IE, the central claim is that careful causal analysis is unnecessary for tasks such as forming simple models of complex devices. Our primary concern is scientific theory formation which calls for a more methodical approach. though it seems that our design could apply to understanding everyday devices. Our work also shares some similarities with the IDS system (Nordhausen & Langley, 1987), which uses experimentation to induce qualitative models. Unlike IDS, our system uses analogy to focus the formation and revision of theories, and directed experiments to test the generated and revised theories.

6. Discussion

Here we have explored the strengths of combining two distinct theory formation and revision systems to form an integrated system based on analogy and experimentation. We showed how such an integration results in a more complete account of the entire scientific discovery process. Theory formation, revision and experimentation are viewed as interrelated and interdependent processes that require each system to postulate well-defined, theoretically motivated queries to use the expertise of the other.

The evaporation example illustrates many finer points of the discovery process. In the evaporation example, a person typically wouldn't generate all possible hypotheses (e.g., evaporation, liquid flow, absorption, vanish, invisible, etc.) and then discriminate between them. The space of hypotheses is made tractable by pruning based on a knowledge of what can happen *and* a knowledge of what is likely to happen (based on analogical precedents). Also, the presence of an experiment generator enabled us to test for the presence of alcohol vapor, rather than having to assume its existence and expend effort on a potentially incorrect hypothesis.

We are still far from programs that truly reflect actual scientific discovery processes. For example, we are strongly bounded by the complexity of qualitative reasoning and must limit explorations to discovering overly simplistic theories. Furthermore, the knowledge bases and reasoning sophistication of existing discovery systems are far too small to escape the "discovering Newton's laws in a day" phenomenon. However, this work takes steps towards realizing the scale and flavor of the task. Furthermore, it has made limitations in the systems clearer and provides a catalyst for further development. Future research in this direction involves modeling an entire cycle of scientific discovery using an example from the history of science such as the formation, revision and, finally, rejection of the caloric theory of heat.

7. Acknowledgements

This work has benefited significantly from discussions with Gerald DeJong, Ken Forbus, Dedre Gentner, and John Collins. This research is supported in part by an IBM Graduate Fellowship to Falkenhainer, by a University of Illinois Cognitive Science / Artificial Intelligence Fellowship to Rajamoney, and by the Office of Naval Research under grants N00014-85-K-0559 and N00014-86-K-0309.

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