Chemical Analogies: Two Kinds of Explanation

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Abstract

Analogies are often used to help provide explanations of unfamiliar phenomena by comparing them to familiar phenomena. Analogical explanations are of two kinds: ones that provide systematic clarification, and ones that give a causal account of why something happened. We describe a theory and implementation of analogical mapping that applies to both kinds of explanation. The theory says that the elements of one analog are mapped onto the elements of another on the basis of structural, semantic, and pragmatic constraints. Our program ACME (Analogical Constraint Mapping Engine) uses localist networks of units representing mapping hypotheses to determine the correspondences between analogs. This paper describes ACME'S application to eight analogies that have been used by chemistry teachers.

1 Analogy and Explanation

Analogies have numerous functions. In problem solving and decision making, analogies to past cases can be used to suggest solutions to new problems [Holyoak & Thagard 1989, Hammond 1986, Kolodner and Simpson 1988, Carbonell 1983, 1986.1. Analogical arguments are sometimes used to reach conclusions, as in the philosophical argument for other minds: since I have a mind, and you are similar to me in numerous respects, I infer that you have a mind also [Thagard 1988]. Analogies have various literary uses, serving to evoke emotions ("Love is a rose"). Finally, analogies can be very valuable in teaching, when an unfamiliar phenomenon is explained in terms of something familiar. For example, we can explain heat flow in terms of water flow, the structure of the atom in terms of the structure of the solar system [Gcntner 1983], or variables in a programming language in terms of boxes that contain objects [Burstein 1986].

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Analogical explanations are of two different kinds, corresponding to two senses of "explain" distinguished by dictionaries:

1. To make plain or clear.
2. To give the reason for or cause of.

We shall call the first kind of explanation *clarifying,* and the second kind *why-answering.* Consider how one might explain the British parliamentary system to an American ignorant of it. The best strategy, at least initially, would be to point out correspondences between the American system and the British:

President - Prime Minister
Congress - Parliament
House of Representatives - House of Commons
Senate - House of Lords

There are problems with this analogy, for example that the Prime Minister is a member of parliament while the President is not a member of congress, but the analogy would give the American a start at understanding the British system. In this case, the analogy serves to make plain the nature of parliament by displaying its systematic correspondences with something that is (for the American) more familiar. A different kind of explanation would be prompted by questions such as "Why was Margaret Thatcher elected Prime Minister in the last British election?" Such why-questions are a request for *causal* explanations: the questioner wants to know what events or situation produced her victory. Sometimes explanations that answer such questions are analogical: Thatcher's victory was like Bush's victory in the 1988 U.S. election, in that the economy was strong and the opposition was not very formidable. The point of this analogy is to suggest how similar phenomena have similar causes.

Both clarifying and why-answering analogical explanations can be found in an interesting section of the *Journal of Chemical Education* called "Applications and Analogies'. This feature consists of letters from chemistry teachers at both high school and college levels who describe analogies that they have found useful in teaching chemistry to their students. For example, one analogy compared flow of energy through molecular motion in a gas to flow of wealth in a population. To learn using the analogies that their teachers give to them, students have to be able to bring the familiar everyday events offered as source analogs into correspondence with the target chemical phenomena. Of thirty-five chemical analogies we have examined, 17 arc clarifying analogies and 18 are why-answering.

A crucial stage in learning by analogy is mapping one analog onto another. In order to use a *source* analog to learn about a *target* analog, people and machines need to be able to determine what elements in the target correspond to what elements in the source. Holyoak and Thagard Tin press] proposed a constraint satisfaction theory of analogical mapping that was applied to numerous examples and used to model the results of several psychological experiments. ACME has now been applied successfully to eight additional analogies selected (as being particularly interesting) from the *Journal of Chemical Education.* Several of these analogies are primarily intended to provide the clarifying kind of explanation, while others have as their primary function explaining *why* something occurs.

2 A Constraint Satisfaction Theory

Holyoak and Thagard fin press] identified three major kinds of constraints that govern how parts of two analogs can be placed in correspondence with each other: semantic similarity, structural consistency, and pragmatic centrality. These constraints are not absolute requirements on successful mappings, but rather arc *pressures* that operate to some degree [Hofstadter 1984].

2.1 Structural Consistency

If we represent analogues as sets of interrelated propositions [Gentner 1983], then structural consistency requires that if a proposition P in the target is in correspondence with a proposition P* in the source, then the predicate and argument(s) of P must each correspond to the respective predicate and argument(s) of P*. If two propositions are mapped, then their constituent predicates and arguments should also map. Two analogues constitute an isomorphism if the mapping between them is structurally consistent and one-to-one. Sensitivity to structural consistency has been a crucial component in virtually all AI models of analogical mapping [e.g., Carbonell 1983; Falkenhainer, Forbus, & Gentner 1986, in press; Kolodner & Simpson 1988; Thagard & Holyoak 1988; Winston 1980]. Gentner's [1983] "systematicity principle" can be interpreted as a special case of structural consistency, in which correspondences between higher-order predicates (those such as "cause", which take propositions as arguments) enforce correspondences involving lower-order relations and their arguments.

2.2 Semantic Similarity

More controversially, Holyoak and Thagard [in press] claimed that mappings should also favor correspondences between elements that are semantically similar. For example, *dog* should tend to map to *cat* more than it does to *house,* since cat and dog are both a kind of animal and a kind of pet. Sophisticated judgments of the semantic similarity of two analogs cannot rely merely on finding identical matches of predicates, but rather require a richer semantics to identify similar concepts. The semantic similarity of concepts in two analogs appears to depend on numerous semantic relations, including:

(1) being represented by the same predicate; and

(2) being connected by semantic relations such as synonymy or kind and part-whole relations.

2.3 Pragmatic Centrality

The constraint of pragmatic centrality favors mappings that help to accomplish the purposes of the analogy. In why-answering explanations, for example, the purpose is generally to give a causal explanation that answers a question or set of questions, so the elements of the propositions to be explained will be particularly important. Hence a mapping should tend to produce correspondences involving the important elements. Numerous AI theorists have argued that causal relevance to goal accomplishment should influence *retrieval* [Winston 1980, 1982; Schank 1982; Carbonell 1983, 1986; Hammond 1986; Kolodner & Simpson 1988]. We maintain that causal relevance should be considered in mapping between analogs as well as in the process of retrieval. Mapping thus involves the simultaneous satisfaction of structural, semantic, and pragmatic constraints.

3 ACME

3.1 Creating a Network of Mapping Hypotheses

The input to ACME (Analogical Constraint Mapping Engine) consists of predicate-calculus representations of the source and target analogs, plus optional information about semantic similarity and pragmatic importance. We assume that a mapping may be computed either from a target analog to a source or vice versa. When given two structures as input, ACME automatically generates a network in accord with the constraints postulated by the theory. The first step in building a mapping network is to construct *mapping units* corresponding to each possible hypothesis about pairings between elements. To limit the number of units formed, correspondences are only allowed between elements of the same basic type: propositions to propositions, n-place predicates to n-place predicates, and objects to objects. ACME constructs units to represent all possible pairings of elements of the same type.

As the units are established, links are formed between them to implement the constraint of structural consistency. All links are symmetrical, with the same weight regardless of direction. All excitatory links have a default excitation weight given by parameter *e.* For predicates that lake more than one argument, the argument mappings support each other. Links are also created between predicate-mapping units and their corresponding argument-mapping units. Each potential correspondence between propositions thus generates an interconnected subnetwork of mutually consistent correspondences between elements of the propositions. After all the units have been formed, inhibitory links with weights equal to a parameter *i* are formed to connect all units that represent alternative mappings for the same element.

In addition to the units representing mapping hypotheses, the network includes two special units. The *semantic unit* is used to convey information about the system's prior assessment of the degree of semantic similarity between each pair of meaningful concepts in the target and source, and the *pragmatic* unit similarly is used to convey information about the pragmatic importance of possible correspondences. The semantic-similarity constraint is enforced by placing excitatory links from the semantic unit to all units representing mappings between predicates. The weights on these links are made proportional to the degree of semantic similarity between the mapped concepts. Similarly, the pragmatic-centrality constraint is represented by weights on links connecting the pragmatic unit to relevant mapping units. Section 4.2 and Figure 1 below provide an example, and a full statement of the algorithms used can be found in Holyoak and Thagard fin press].

3.2 Running the Network

The manner in which the network is run to arrive at a solution is a straightforward application of constraint-satisfaction methods that have been investigated extensively in other applications (see Rumclhart and McClelland 1986]. To initialize the network, the activation levels of the semantic and pragmatic units are fixed at 1 and the activations of all other units are set to 0. On each cycle of activity, all units (except the semantic and pragmatic units) have their activation levels updated on the basis of the activation levels and weights associated with neighboring units and links. The updating procedure is based on that suggested by Grossberg [1978]. The activation level of unit) on cycle *t+1* is given by:

$$a_j(t+1) = a_j(t)(1-d) + \qquad (1)$$

$$enet_j(max - a_j(t)) + inet_j(a_j(t) - min).$$

Here d is a decay parameter, $enet_j$ is the net excitatory input, and $inet_j$ is the net inhibitory input (a negative number), with minimum activation min=-1 and maximum activation max=1. Inputs are determined by the equations:

$$enet_j=\sum_i w_{ij}o_i(t) \text{ for } w_{ij}>0; \text{ and} \qquad (2)$$

$$inet_j=\sum_i w_{ij}o_i(t) \text{ for } w_{ij}<0. \qquad (3)$$

In equations 2 and 3, $o_i(t)$ is the output on cycle t of unit i, set by:

$$o_i(t)=\max(a_i(t), 0). \qquad (4)$$

Updating continues until all units have reached asymptote, that is, a cycle is reached at which the activation change of each unit is less than a specified value, typically .001.

3.3 Comparison With Other Models of Analogy

As we noted earlier, many previous simulation models of analogical mapping have been proposed [see Hall, in press; Thagard, 1988]. Other models have included structural, semantic, and pragmatic constraints on mapping, but no single model has integrated these constraints as ACME does. The most closely related previous simulation is the SME program, which was developed as an implementation of Gentner's structure-mapping theory [Falkenhainer et al., 1986; Gentner, 1983, 1989].* ACME and SME have several important similarities. Both models derive a global "best" mapping from a set of constituent hypotheses about element correspondences (the mapping units of ACME and the "match hypotheses" of SME). Both programs operate on predicate-calculus representations of analogs, and both emphasize the role of proposition mappings in enforcing mappings between corresponding elements of the propositions.

ACME follows SME in using constraints of structural consistency and one-to-one mapping, but there are notable differences. Whereas SME insists on mappings that are one-to-one, ACME operates with pressures that prefer but need not necessarily produce such mappings. ACME treats isomorphism as a separate constraint from semantic similarity: Whereas SME requires multi-place relations to be identical in order to be mapped, ACME allows mappings between relations with no similarity beyond having the same number of arguments. More generally, ACME includes semantic and pragmatic constraints on the mapping component, as well as purely structural constraints. ACME prefers mappings between elements that are semantically similar, whereas SME excludes such information as relevant only to stages of analogy outside mapping. To implement the constraint of pragmatic centrality, ACME allows preferences for "presumed" mappings and for mappings involving "important" elements.

Mapping is at least implicitly part of every analogy program, but space restrictions prevent us from comparing ACME with models that have been proposed by, for example, Winston [1980, 1982], Hofstadter [1984], Anderson and Thompson [1989], Kolodner and Simpson [1988], Hammond [1986], Carbonell [1982, 1983], and Burstein [1986]. For analogies restricted to a single domain in which the same predicates and arguments turn up in both structures to be mapped, mapping becomes a simple special case of the more complex processes used by ACME and SME for cross-domain analogies.

4 Application of ACME to Chemical Analogies

4.1 Eight Analogies

ACME hits been successfully applied to a total of eight analogies from the *Journal of Chemical Education*. A

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[1] SME runs in several different modes. Our comparison here is with SME running in the mode that implements Gentner's structure-mapping theory.

few of these were quite simple, whereas others involved numerous propositions and complicated mappings. Here is a list of the analogies with a brief description of each. The first 5 are why-answering analogies, whereas the last 3 are clarifying.

(1) Leveling effect of solvents and opening jars [Macomber 1984]. Students have difficulty understanding how the basicity of a solvent can affect the apparent acidity of a compound. This analogy compares strongly and weakly basic solvents to a father and son who differ in their abilities to open stuck jars: the father can open some jars that are too tightly stuck for the son to open, just as a strongly basic solvent can dissociate weaker acids (that have protons bound tightly) than can a weakly basic solvent.

(2) Chemical bonds and tug of war [Tsaperlis 1984]. This is intended to help students understand how atoms are held together. Atoms with bonds between them are compared to two people playing tug of war with a rope. The atoms are bonded together because they compete for electrons, just as the people are held together because they compete for the rope.

(3) Gas chromatography and store escalators [Starkey 1986]. Students have the misconception that the separation of a mixture of compounds in a gas chromatography column involves different lengths of time that each compound spends in the mobile (gas) phase, whereas the difference really comes in the stationary (liquid) phase. The gas column is compared to a store with escalators, where shoppers enter at the first floor and make their way up eight floors to the top. The different length of time it takes them to get to the top does not depend on the amount of time they spend in transit on the escalators, but only on how much time they spend shopping on the floors.

(4) Distribution of molecular velocities and distribution of wealth [White 1981a]. This analogy compares the distribution of molecular velocities to the distribution of money. Just as a series of financial gains can lead a millionaire to have an action-filled life, so a series of collisions can cause a molecule to gain enough energy to react.

(5) Soluble vs. insoluble mixtures and marble/magnet mixtures [Kjonaas 1984]. Mixing polar molecules such as water and non-polar molecules such as oil produces an insoluble mixture, just as putting marbles and magnets together fails to produce a homogeneous mixture because the magnets stick together.

(6) Chiral molecules and people's hands [Richardson 1982]. How chiral molecules react to one another is compared to how people are more easily able to shake the right hands of other people with their right hands than with their left hands. There is no attempt here to explain *why* molecules have these relationships, only to point out systematic correspondences with human hands.

(7) Entropy as degree of disorder and classroom attire [White 1981b]. In order to convey an understanding of entropy, this analogy considers a classroom in which every member owns a pair of blue jeans and a white shirt or blouse, as well as other clothes. It is highly improbable that the class will end up in a uniform state with all of them wearing the same color jeans and shirt on a given day. No explanation is given of why order and disorder arise in chemical phenomena.

(8) Reactions yields and voter turnout [Rocha-Filho 1986]. Just as in an election only some of the members of the electorate actually vote, so in a chemical reaction the actual yield is often less than the theoretical yield. No explanation is given of why the theoretical yield is less; the point of the analogy is merely to clarify the discrepancy in reactions by relating it to the more familiar discrepancy in elections.

In order to apply ACME to them, each of these analogies was formalized in predicate calculus. The resulting representations were then used by ACME to generate constraint networks. Table 1 gives information about the results of running each analogy. It displays for each analogy the total number of propositions used to represent each pair of analogs, the number of units created by the network, the number of links set up, the number of cycles of updating it took before ACME came up with the correct mapping

Table 1: Chemical Analogies

analogy	propositions	units	links	cycles to settle	cycles to success	excitation ceiling	inhibition floor
(1) Solvents/jars	36	274	3119	50	8	.07	-.08
(2) Bonds/tug of war	26	126	964	43	5	.1	-.09
(3) Gas/escalators	16	88	551	47	5	.16	-.05
(4) Molecules/wealth	30	207	1778	47	5	.09	-.05
(5) Soluble/magnet	24	137	1127	77	14	.18	-.06
(6) Molecules/hands	24	176	1903	45	9	.1	-.12
(7) Entropy/attire	16	18	50	63	4	.5	-.03
(8) Reaction/election	6	15	35	64	3	.4	-.01

(when the unit representing the correct mapping for each predicate had higher activation than competing units), the number of cycles it took the network to settle (when every unit had reached asymptote), and two sensitivity measures explained in section 4.3.

4.2 A Sample Network

Most of the networks produced in these examples are too complex to show in a one-page figure, but Figure 1 shows the network produced for analogy (8) which was by far the simplest, requiring only 15 units and 35 links. The input for this analogy consisted of only 3 propositions per structure:

Election
(electorate (number-possible-voters) s1)
(turnout (number-actual-voters) s2)
(greater (number-possible-voters number-actual-voters) s3)

Reaction
(theoretical-yield (number-reactant-molecules) t1)
(actual-yield (number-product-molecules) t2)
(greater (number-reactant-molecules number-product-molecules) t3)

In this case, but not in all the others, the structures are isomorphic. The last element in the list is the name of the proposition. For conciseness, Figure 1 uses the abbreviations EL, TU, G, TY, and AY for the predicates above, and pv, av, rm, and pm for the objects. For example, EL=TY is the unit that represents the hypothesis that *electorate* corresponds to *theoretical-yield.* Excitatory links are shown by solid lines, while inhibitory links are shown by dotted lines.

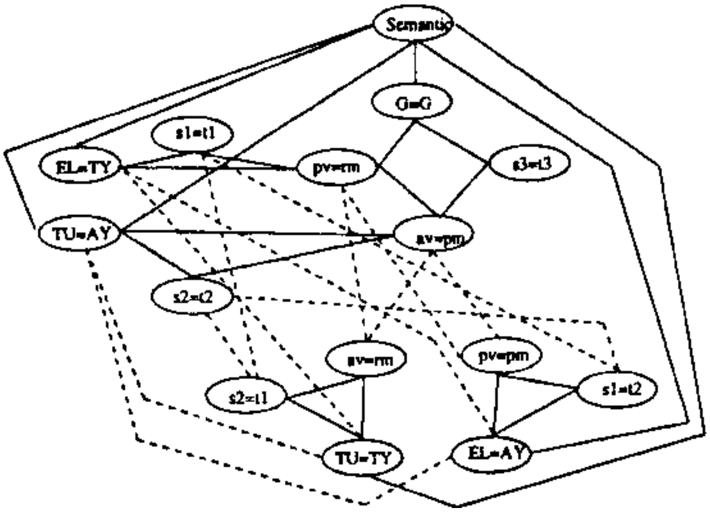

Figure 1.
Network Constructed for the Reaction/Election Analogy

4.3 Sensitivity Analyses

All of the simulations reported here have used the same parameter values: .05 for excitation. -.2 for inhibition, and .1 for decay. In general, lowering excitation and making inhibition closer to 0 tends to prolong settling time. Increasing decay tends to flatten the activation curves, both positive and negative, keeping them closer to 0. Varying excitation and inhibition systematically reveals that there is a critical value for each. Table 2 lists excitation ceilings and inhibition floors for the four major examples. The excitation ceilings are the maximum values that excitation can have without the networks requiring more than 100 cycles to settle; inhibition here is constant at the default value of -.2. The inhibition floors are the minimum values that inhibition must have to de-activate units representing inferior hypotheses; excitation here is constant at the default value of .05. The excitation ceiling and the inhibition floor indicate the most important respects in which quantitative parameter changes in ACME have qualitative effects.

Analogical mapping is highly sensitive to representational matters, but ACME's success on the chemical analogies does not depend on our particular encodings. To test the representational sensitivity of our inputs, we amalgamated the solvents/jars analogy with the bondsAug of war analogy and mapped a combined solvents + bonds structure with a combined jars + tug of war structure. The resulting network had 700 units and 11,788 links, but settled in 52 cycles, only slightly more slowly than the networks used in the original analogies. ACME found the same mappings for the solvents and bonds predicates that it did in the original runs, showing that the additional representations did not impede its ability to find correct mappings.[2]

5 Conclusion

In sum, the 8 chemical analogies have provided interesting additional applications of the constraint satisfaction theory of analogical mapping. There are more than twenty analogies in the *Journal of Chemical Education* that we have not yet attempted to model. It will be interesting to see if they highlight additional extensions needed to our theory and program. The most important future work planned for ACME is to integrate it with ARCS, a program for modeling the *retrieval* of analogs [Thagard, Holyoak, Nelson, & Gochfeld, 1989]. Retrieval of a source analog from a target has also proven understandable in terms of satisfaction of a variety of constraints. The psychological evidence suggests, however, that retrieval depends more on semantic similarity and less on structural consistency than

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[2] Holyoak and Thagard tin press] show that the space complexity of ACME is $0(n^4)$, considering number of links created as a function of number of propositions in the input representations. Experiments have shown that cycles to settle does not tend to increase with size of network.

does mapping, so ARCS differs from ACME in giving a much bigger role to semantics.

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