APPROXIMATION IN MATHEMATICAL DOMAINS

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ABSTRACT

Explanation-based learning is accomplished through the generalization of an explanation produced by analysis of a single example. A theory of the domain is utilized in generating the explanation. However, problems arise when the domain theory is intractable. Simplifications must be made in order to make the problem tractable. Well-founded simplifications based on our real world knowledge are termed *approximations.* This paper discusses how approximations can be used to deal with the intractable domain problem in mathematical domains. The approximation method strongly supports the use of a mix of quantitative and qualitative reasoning over either a purely quantitative or qualitative approach. The approximation technique is demonstrated on one of the examples which has been implemented in the chemistry domain.

1. Introduction

Explanation-based learning makes use of domain theory to construct an explanation for a single observed example. The explanation is then generalized so the generalized concept can be used in future problem-solving. Explanation-based learning (EBL) is currently the subject of much research. Many EBL systems have been constructed and work is proceeding in capturing a domain independent generalization technique [1-3].

EBL depends on the ability to construct an explanation for the example. This becomes difficult when we are dealing with an imperfect domain theory [l. 2. 4. 5]. Mitchell outlines three types of imperfect theories: those which are inconsistent, those which are incomplete, and those which are intractable. Our focus in this paper is with intractable theory in mathematical domains.

An intractable problem is one which is very difficult to solve where, because of the great number of rules and/or ways they can be applied, we do not quickly reach the goal. Many real-world problems are of this type. For instance, consider trying to explain why the unemployment rate changed. It is not possible to construct an exact explanation. There will always be further order causations which must be considered inconsequential. Economic theories explaining the change are necessarily approximate. Furthermore, due to the approximate nature of **the** explanations, many plausible explanations are possible as is evidenced by the variety of economic views.

In mathmatical domains, where a set of exact rules is available, we encounter intractability due to the great number of possible applications of the rules. Chemists who work in chemical kinetics very often need lo solve very complicated differential equations. Frequently, the equations, as they stand, along with **the** set of mathematical operators characterize an intractable *problem* as *discussed* above. Chemists *proceed* to a solution in the only way they can: by applying their common-sense knowledge to form approximations to the original equations.

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Approximation is an attractive technique for use in mathematical problem solving because it allows us to solve intractable problems and at the same time can frequently lead to more efficient solutions to tractable problems which don't need a precise answer. In many cases the exact solution is no more desirable than an approximate one. In a laboratory situation, results might only be 95% accurate due to experimental error. Therefore, when calculations are performed they need not have less than 5% error. In fact, no more than 95% accuracy can be claimed.

This paper investigates how approximation can be used to produce explanations to examples in mathematical domains. First, we discuss the method by which approximations can be made. Integral in this discussion is how quantitative and qualitative reasoning are used. Next, a chemistry example is introduced which illustrates how the method is applied. Last, conclusions and future research directions are discussed.

2. How Are Approximations Made?

Approximations can be made when one has a body of qualitative knowledge about a domain. This is really what we refer to as common-sense knowledge. The knowledge doesn't need to be quantitatively precise, only to enable inferences which can help us to solve the problem.

Many researchers have addressed the apparent dichotomy between qualitative and quantitative knowledge. One of these researchers. Johan dekleer. has shown how the two types of knowledge can be used together in the domain of classical mechanics [6]. In deKleer's approach, the first step is *envisioning* which is purely qualitative. Given a mechanics problem, this would entail enumerating the possibilities of what *could* happen. When the problem is a simple one. envisioning alone may solve the problem by enumerating only one possible outcome. In more complex problems, the number of envisionments is much greater. Here, dekleer uses quantitative knowledge to help disambiguate between possible envisionments.

Clearly, the envisioning process can be an expensive one for complex problems. For highly mathematical problems, the quantitative analysis plays a greater role in problem-solving. Our approach is to start with a quantitative representation of the problem. The exact quantitative representation is relaxed into an approximate representation using qualitative domain rules and magnitude reasoning.

Explanations can be constructed at several levels of abstraction. Doyle addresses the case when we must refine an explanation to a less abstract level due to inconsistencies that arise at the current level [7], Tadepalli indicates the importance of moving to more abstract levels (through approximation) as a method of generating explanations in intractable domains [8]. We will use the latter method: one which takes us from a lesser to a greater abstract representation.

In a mathematical domain, the inferences we make using our qualitative knowledge can lead us to consider certain quantities negligible with respect to other quantities. We can then modify our formulae on the basis of the determined negligible quantities to arrive at an approximate set of formulae. For example, a variable can be neglected in a sum formula if it can be considered negligible with respect to all the other quantities in the formula. Figure 1 illustrates this:

Given:

$$A = B + C$$

Then:

$$B << A \;\&\; B << C \rightarrow A \approx C$$

$$C << A \;\&\; C << B \rightarrow A \approx B$$

$$A << B \;\&\; A << C \rightarrow B \approx -C$$

Figure 1: Approximation Within A Sum

There are many variations on this rule. They all ultimately involve neglecting a quantity because it is insignificant in relation to other quantities in a sum. Several researchers have developed systems which perform order of magnitude reasoning similar to that illustrated above. Recent papers include [9] and [10]. We will apply this type of reasoning to the introduction of approximations.

Figure 2 shows the method by which approximation is used in solving mathematical problems. The knowledge the system uses in solving the problem has both domain dependent and domain independent components. The domain independent portion is pertinent to any examples which involve mathematical reasoning. Such problem solving skills rely on both quantitative and qualitative knowledge. There has been a tendency in past work to separate these. To use approximation in mathematical domains, one must frequently use both types of reasoning.

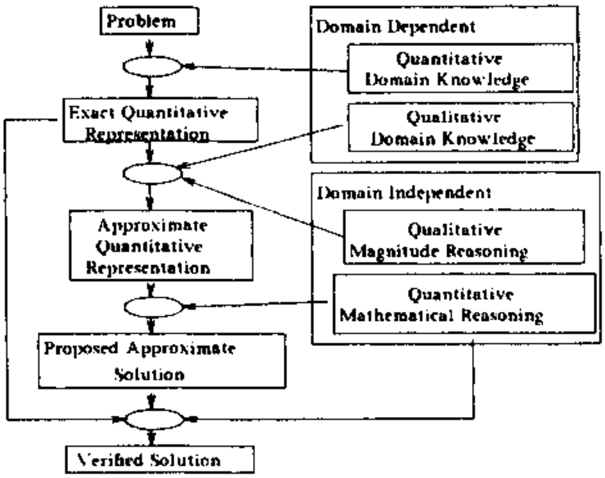

Figure 2: The Approximation Method

When purely quantitative reasoning is used, many complex problems cant be solved. The system must take full advantage of the information available, including less exact qualitative information which can help it to simplify the situation.

Purely qualitative reasoning can also fail. The quantitative equations representing the problem contain much information. Representing everything in a qualitative fashion is not always desirable and can lead to a large number of envisionments which must be disambiguated.

One starts with a representation of the problem statement.[1] This representation can be translated into a quantitative representation which consists primarily of equations describing the situation as well as the expression or expressions which we are trying to find. Such a translation makes use of quantitative domain knowledge which explains exactly how quantities are related. Had we decided not to use approximations, we would attempt to use our quantitative mathematical reasoning abilities to solve the problem. If the problem is a tractable one. this will lead to a solution, although it may require much effort. If the problem is intractable, it may be impossible to reach the solution in this way.[2] So. our next step is to analyze our quantitative representation to see if simplifications can be made. This means using techniques like qualitative magnitude reasoning in conjunction with our qualitative domain knowledge to introduce approximations. The result is a simplified set of equations, due to negligible terms having been eliminated. We bring our quantitative mathematical reasoning to bear on the problem to arrive at an approximate solution. In many mathematical examples, it is possible to check the validity of our approximations. The last step is to use our mathematical reasoning in conjunction with the original exact quantitative representation to calculate error. If the error is acceptable, our solution is complete.[3] In mathematical domains, this ability to learn about the validity of our approximation is an especially important tool.

3. An Example: Acids In Solution

Now, let us consider how this technique is applied. Here is an example, which has been fully implemented, involving an analysis of the effects of adding an acid to water. This chemistry problem, taken from [11, p. 113], is:

> Find the concentrations of all species in a 0.010 molar solution of acetic acid with $K_a = 1.75 \times 10^{-5}$. The equilibrium constant for water is $K_w = 10^{-14}$. The *OH* ion concentration in pure water is C_w — 10 .

This type of problem can become intractable if we introduce more ions into the solution but. for purposes of illustration, we present this simplified version. This example uses straightforward inferences, clearly shows how one's qualitative assumptions effect the resulting solution, and shows a quantitative verification of the assumptions. In the problem, the following two equilibria are known to be present:

$$HAc \overset{K_a}{\rightleftharpoons} H^+ + Ac^- \qquad \text{(E1)}$$

$$H_2O \overset{K_w}{\rightleftharpoons} H^+ + OH^- \qquad \text{(E2)}$$

Equilibrium E1 represents the dissociation of Acetic Acid (HAc) into H^+ and *Ac* - ions in solution. What complicates the problem is that equilibrium E2 is also present and represents the dissociation of water (H_2O) into H^+ and *OH-* ions. The constants K_a and K_w are called equilibrium constants. They reflect how far the equilibrium is shifted to the left or right. This concept of an equilibrium can be represented by a quantitative formula. The respective quantitative relationships for E1 and E2 are (brackets denote concentrations):

$$[H^+][Ac^-] = K_a[HAc] \qquad \text{(Q1)}$$

$$[H^+][OH^-] = K_w \qquad \text{(Q2)}$$

[1] We will not address the translation from natural language to the representation.

[2] Usually one would resort to numeric methods some of which are actually repeated approximations.

[3] If necessary, we can use this feedback in a loop to arrive at the technique of successive approximations whereby our error gets smaller on every iteration until it is within the desired bounds.

In Q2. $[H_2O]$ doesn't appear because, since the concentration of water is assumed to be constant, it has already been included in K_w. Two more equations need to be written: the charge balance equation and the mass balance equation. The charge balance equation equates the total amount of positive charge with the total amount of negative charge:

$$[H^+] = [Ac^-] + [OH^-] \qquad (Q3)$$

The mass balance equation illustrates that if we start with C_0 moles/liter of HAc. that acetate (Ac) is conserved after some of the HAc has formed Ac ~.

$$[HAc] + [Ac^-] = C_0 \qquad (Q4)$$

With a knowledge of equations Q1 through Q4 and the constants K_a. K_w. C_0 and C_w. a cubic equation can be developed which will lead to an exact solution. However, for most purposes, only an approximation is necessary. For those who utilize their commonsense knowledge of chemistry, the approximation is far easier and yields results far more quickly than the exact solution. Had we considered a problem with more equilibria, the order of the exact equation would have increased enough to make this an intractable problem.

The commonsense knowledge which is applied to this problem is represented in the form of inferences. The following two rules from our set of chemistry domain rules are pertinent to this problem: problem:

(Rule 1)
IF the acid is present at a much greater concentration than I(r^7 Molar. THEN [OH-] will be negligible compared to all other species.

(Rule 2)
IF the acid is a weak acid. THEN $[Ac^-] << [HAc]$. This is because weak acids dissociate very little.

These rules tells us what to expect the relationship between the quantities to be based on the strength of the acid and/or its concentration. If we knew neither, these inference rules would not help us to make any approximations. But, in this specific example, we now do know that Acetic acid is commonly considered to be a weak acid. Furthermore. 0.010 is far greater than 1(>-^{7}. This means that rules 1 and 2 apply, yielding: \OH-] negligible with respect to everything and [Ac~]«[HAc }. This reduces equations Q3 and Q4 to:

$$[H^+] = [Ac^-] \qquad (Q3A)$$

$$[HAc] = C_0 = 0.010 \qquad (Q4A)$$

Now the system proceeds using its basic quantitative knowledge to much more easily solve lor the unknowns. Combining equations Q1. Q3A. and Q4A we arrive at:

$$[H^+] = \sqrt{K_a C_0} = 4.18x\,10^{-4} \qquad (Q5A)$$

Q2 and Q5A give:

$$[OH^-] = \frac{K_w}{\sqrt{K_a C_0}} = 2.39x\,10^{-11} \qquad (Q6A)$$

03. Q5A.andQ6A give:

$$[Ac^-] = \sqrt{K_a C_0} - \frac{K_w}{\sqrt{K_a C_0}} = 4.18x\,10^{-4}$$

Now we have expressions for all the unknowns. The expressions are all based on our initial assumptions: the strength of the acid, and the correctness of our inference rules. In problems like these, we can verify the correctness of our assumptions. We use equation Q4:

$$[HAc] + [Ac^-] = 4.18x\,10^{-4} + 1.00x\,10^{-2} = C_0 = 1.04x\,10^{-2}$$

The approximation is good to within 5%. We can now express our error in terms of K_a. K_w. and C_0 as follows:

$$Error = \frac{\sqrt{K_a C_0} - \frac{K_w}{\sqrt{K_a C_0}}}{C_0} \qquad (Phi)$$

Once the approximate solution has been constructed, the solution structure is generalized using the EGGS generalization technique [3] to produce rules like the following

Learned Rule For Hydrogen Ion Concentration
After Adding ?ha To Water:

```
(dissoc-const water ?kw) & (dissoc-const ?ha ?ka) & (acid ?ha) &
(strength ?ha weak) & (conc ?ha ?c0) and (> > ?c0 (expt 10 -7)) &
(pos-ion ?ha ?h) & (neg-ion ?ha ?a) & (pos ion water ?h) &
(neg-ion water ?oh)
==> (aqueous-conc ?h (sqrt (* ?ka ?c0)))
```

Aitnougn not shown in the above rule, the error estimation form shown in PE1 can be incorporated into the precondition of the rule to check it the rule meets the system's specified accuracy criterion.

4. Conclusions

A method has been proposed that shows how approximation can be used to overcome obstacles in mathematical problem solving [12]. Powerful techniques like these permit solutions to otherwise intractable problems and can facilitate efficient solution to many less difficult problems. One advantage of using an approximation technique like this in a mathematical domain is our ability to reason about the correctness of the approximation. Any flaws in our original domain dependent qualitative rules become immediately evident when we attempt to verily the solution. We can also more accurately determine future applicability of the formula.

Many issues have yet to be addressed. This paper has discussed how approximation takes place in highly mathematical domains. There are many other domains in which approximation can be used to deal with intractability Work is underway in developing a system which generates plausible explanations for observed events An explanation is selected for generalization but difficulties with the new generalized rule will trigger generation of a new plausible explanation for the observations.

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