APPROXIMATION IN MATHEMATICAL DOMAINS

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Approximation in Mathematical Domains

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ABSTRACT

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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 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.

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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 [Mitchell83][Mitchell85][Mooney85][O'Rorke84][Winston83] and work is proceeding in capturing a domain independent generalization technique [Mitchell86][DeJong86][Mooney86].

EBL depends on the ability to construct an explanation for the example. This becomes difficult when we are dealing with an imperfect domain theory [Mitchell86][DeJong86][Rajamoney87][Chien87]. 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, because the operators can be applied in many ways and do not take us quickly to our goal. A game of chess exemplifies the intractable problem. We can relatively easily define the rules of how to play chess but actually playing out a game to reach a win is considerably more difficult. Each move is relatively easily made and takes us a short distance toward our goal. The challenge is in choosing the correct move. Planning is much more difficult with an intractable theory.

In this paper, we introduce the method of approximation to handle examples in intractable domains. For example, chemists who work in chemical kinetics very often need to 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.

Approximation is an attractive technique for use in problem-solving because the exact solution is often no more desirable than an approximate one. For example, 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.

Sometimes, in more tractable problems, when complete accuracy is not needed, the approximate solution is favored over the exact solution for efficiency reasons. If you need a computer subroutine to draw a line on a computer display, you might first start by using the equation for a line. By plotting the line on a discrete set of points on the display, you are forced to approximate the line. Use of the line equation involves performing multiplications and divisions for each point plotted and is relatively slow. Good approximate line drawing routines involve no multiplications or divisions as the line is drawn, just integer arithmetic. The lines are drawn quickly because they need only be as accurate as the display device. Use of a specific approximation can be far better than using the exact technique when less precision is required.

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

quantitatively precise; only to enable inferences which can help us to solve the problem. Qualitative reasoning is currently a popular research topic.¹

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 [de Kleer75]. In deKleer's approach, the first step is envisioning. 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 [Doyle86]. Tadepalli indicates the importance of moving to more abstract levels (through approximation) as a method of generating explanations in intractable domains [Tadepalli85]. 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. The following formula illustrates this:

\[
\begin{align*}
\text{Given:} & \quad A = B + C \\
\text{Then:} & \quad B \ll A \land B \ll C \Rightarrow A \approx C \\
& \quad C \ll A \land C \ll B \Rightarrow A \approx B \\
& \quad A \ll B \land A \ll C \Rightarrow B \approx -C \\
\text{Approximation Within A Sum}
\end{align*}
\]

There are many variations on this rule such as the one illustrated below. They all ultimately involve neglecting a quantity because it is insignificant in relation to other quantities in a sum.

\[
\begin{align*}
\text{Given:} & \quad A + C \\
\text{Then:} & \quad A > 1 \land B \ll C \Rightarrow A + C \approx A \\
\text{Another Example Of Approximation}
\end{align*}
\]

¹ For more information about this area, a good source is [Forbus84].
Several researchers have developed systems which perform order of magnitude reasoning similar to that illustrated above. Recent papers include [Raiman86] and [Simmons86]. We will apply this type of reasoning to the introduction of approximations.

The figure below shows the method by which approximation is used in solving mathematical problems. The knowledge we use 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.

When purely quantitative reasoning is used, many complex problems can't be solved. We must take full advantage of the information available to us, including less exact qualitative information which can help us in simplifying 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 envisionsments which must be disambiguated.

The Approximation Method
One starts with a representation of the problem statement. 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. 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. Usually, we will be able to use our common-sense knowledge to simplify things. Now, we have 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. It is important, however, to check the validity of our approximation. 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. 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 [Butler64, p.113], is:

Find the concentrations of all species in a 0.010 molar solution of acetic acids with

\[ K_a = 1.75 \times 10^{-5} \]

**Constants**

- **Equilibrium Constants**
  - **For Acetic Acid**
  - **Equilibrium Constant**
    - **For Water**
  - **Initial Acetic Acid**
    - **Concentration**
  - **OH− Ion Concentration**
    - **In Pure Water**

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 methods, some of which are really repeated approximations.

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2 We won't address translating from natural language to the representation.

3 Usually one would resort to numeric methods some of which are really repeated approximations.

4 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.
Approximation in Mathematical Domains

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:

\[ \text{HAc} \rightleftharpoons \text{H}^+ + \text{Ac}^- \]  
\[ \text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^- \]

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\(_2\)O) 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:

\[ [\text{H}^+][\text{Ac}^-] = K_a[\text{HAc}] \]  
\[ [\text{H}^+][\text{OH}^-] = K_w \]

In Q2, \([\text{H}_2\text{O}]\) 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:

\[ [\text{H}^+] = [\text{Ac}^-] + [\text{OH}^-] \]

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\(^-\):

\[ [\text{HAc}] + [\text{Ac}^-] = C_0 \]

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 common-sense 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 are pertinent to this class of problem:

(Rule 1)

IF the acid is present at a much greater concentration than \( 10^{-7} \) Molar, THEN [OH\(^-\)] will be negligible compared to all other species.

(Rule 2)

IF the acid is a weak acid, THEN [Ac\(^-\)] \( \ll \) [HAc]. This is because weak acids dissociate very little.

(Rule 3)

IF the acid is a strong acid, THEN [HAc] will be negligible compared to all other species. This is because strong acids nearly totally dissociate.
Approximation in Mathematical Domains

(Rule 4) If the acid's concentration is close to $10^{-7}$ Molar, THEN \([\text{HAc}]\) will be negligible compared to all other species. This is because there was so little of the acid, that it all dissociated.

(Rule 5) If the acid's concentration is much less than $10^{-7}$ Molar, THEN \([\text{Ac}^-] \ll [\text{H}^+]\) and \([\text{Ac}^-] \ll [\text{OH}^-]\). If the acid is present in small enough quantities, the water equilibria dominates.

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 $10^{-7}$. This means that rules 1 and 2 apply, yielding: \([\text{OH}^-]\) negligible with respect to everything and \([\text{Ac}^-] \ll [\text{HAc}]\). This reduces equations Q3 and Q4 to:

\[
[\text{H}^+] = [\text{Ac}^-] \quad \text{(Q3A)}
\]
\[
[\text{HAc}] = C_0 = 0.010 \quad \text{(Q4A)}
\]

Combining equations Q1, Q3A, and Q4A we arrive at:

\[
[\text{H}^+] = \sqrt{K_a C_0} = 4.18 \times 10^{-4} \quad \text{(Q5A)}
\]

Q2 and Q5A give:

\[
[\text{OH}^-] = \frac{K_w}{\sqrt{K_a C_0}} = 2.39 \times 10^{-11} \quad \text{(Q6A)}
\]

Q3, Q5A, and Q6A give:

\[
[\text{Ac}^-] = \sqrt{K_a C_0} - \frac{K_w}{\sqrt{K_a C_0}} = 4.18 \times 10^{-4}
\]

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:

\[
[\text{HAc}] + [\text{Ac}^-] = 4.18 \times 10^{-4} + 1.00 \times 10^{-2} = C_0 = 1.04 \times 10^{-2}
\]

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:

\[
\frac{\sqrt{K_a C_0} - \frac{K_w}{\sqrt{K_a C_0}}}{C_0} = \text{Error} \quad \text{(PE1)}
\]

Once the approximate solution has been constructed, the solution structure is generalized using the EGGS generalization technique [Mooney86] to produce rules like the
Approximation in Mathematical Domains

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)
(> ?c0 (expt 10 -7))
(pos-ion ?ha ?h)
(neg-ion ?ha ?a)
(pos-ion water ?h)
(neg-ion water ?oh)
```

Although not shown in the above rule, the error estimation form shown in PEI can be incorporated into the precondition of the rule to check if 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 [Shavlik85]. 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 verify 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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References


Approximation in Mathematical Domains

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