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An optimization approach to order of magnitude reasoning

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Abstract

An approach for transforming the order of magnitude relation between two variables into an algebraic equality or inequality constraint is provided. In order to derive the order of magnitude relation between any two variables, a nonlinear optimization problem is solved for the minimum and maximum values of the ratio between the two variables, subject to two classes of constraints. The first class of constraints corresponds to the quantitative model and the second class of constraints corresponds to the qualitative model. The optimization approach is shown to provide more precise inferences as compared to the conventional constraint satisfaction approaches. Moreover, this approach provides a crucial step in developing unified frameworks that allow the incorporation of qualitative information at various levels of abstraction into numerical frameworks used for reasoning with quantitative models.

Keywords: O(M) Reasoning; AI and Optimization

1. INTRODUCTION

Design and analysis of engineering systems or devices is based on both quantitative and qualitative information. Quantitative information is based on the first principles of the science that underlie physical processes and are described in terms of systems of equations parameterized by physical constants. For example, chemical processes are described in terms of rate equations and various thermodynamic correlations. Usually the physical constants that appear in these equations are known with great numerical accuracy. In general, a wide variety of numerical techniques are used for making inferences with such quantitative information.

On the other hand, qualitative information is of a heuristic nature and is largely informed by prior experience and expert judgment regarding the choices that lead to acceptable outcomes. Such information is characterized by Boolean logic or by algebraic equations with partial knowledge such as signs of quantities, relative orders of magnitude of quantities, and interval values for quantities. The last decade has seen much effort toward developing mathematical representations for such qualitative information using various forms of multivalued logics. Computationally, Boolean logical inference is based on resolution theorem proving. Representations for order of magnitude relations are similar to multivalued logics, and constraint satisfaction approaches such as assumption-based truth maintenance systems (ATMS) are used for inference.

The ability to integrate both quantitative and qualitative knowledge in a common framework is desirable since it would allow us to bring knowledge from both first principles and experience to the problem at hand. Some work has been done toward integrating qualitative knowledge expressed in Boolean logic with quantitative information expressed in terms of linear constraints. The Boolean logic is transformed into a set of mathematical expressions using integer arithmetic and combined with the linear constraints in a mixed integer linear programming framework. However, in many engineering problems the qualitative information is in terms of relative orders of magnitude or intervals, and there does not exist a methodological approach to integrate such information with general quantitative models expressed in terms of linear/nonlinear constraints.

In this article we develop an approach for integrating qualitative order of magnitude information with quantitative information expressed as linear/nonlinear con-

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straints in a unified nonlinear programming framework. The order of magnitude relation between any two variables is transformed into an equality constraint by introducing a variable r that is the ratio of the two variables. Based on the order of magnitude relation, the upper and lower boundaries for the ratio r are specified. In order to derive the order of magnitude relation between any two variables, a nonlinear optimization problem for the minimum and maximum values of the ratio of these two variables is solved, subject to two classes of constraints. The first class of constraints corresponds to the quantitative model and is derived from the first principles that underlie the process under consideration, and the second class of constraints corresponds to the qualitative model that is derived from heuristic knowledge.

The rest of the article is organized as follows. Section 2 provides an overview of the various mathematical representations that have been developed in the qualitative reasoning literature for expressing partial information such as signs of quantities and order of magnitude information. A brief description of the integrating framework for Boolean logic with linear constraints is also provided. Section 3 describes an approach we have developed to transform order of magnitude relations into a set of equality and inequality constraints. These constraints along with the quantitative information are then used in an optimization framework to derive order of magnitude relations between variables of interest. Section 4 presents three examples to illustrate this approach. Two of the examples are borrowed from the qualitative reasoning literature, and a new example that uses notions from qualitative stability is introduced. The optimization approach is shown to provide more precise inferences as compared to the conventional approaches for order of magnitude reasoning. Section 5 presents a discussion on the implications of this work. Some thoughts regarding how to integrate qualitative information of all forms (Boolean logic and order of magnitude relations) with quantitative information using a mixed integer nonlinear programming framework (MINLP) are presented. Section 6 presents conclusions of this work.

2. PREVIOUS WORK

In engineering applications, qualitative information at various levels of detail are encountered. Boolean models are often used to express the existence of constraints between relevant variables. For example, Boolean models are commonly used in fault diagnosis applications, especially in the context of digital circuits to describe cause–effect relations between variables/components of a physical device. Such models are useful for the generation of hypotheses that explain observed malfunctions (Hamscher, 1991). Several examples of the use of propositional logic in process synthesis in chemical engineering are provided by Raman and Grossman (1991). However, in a large class of engineering problems that deal with continuous process variables, more detailed information such as signs of variables and the direction in which each variable affects another is also available. For example, fault simulation of helicopter engines (Subrahmanian et al., 1988), space shuttle main engine (Hoffman et al., 1992), and fault simulation in process engineering applications (Oyeleye & Kramer, 1987; Venkatasubrahmanian & Rich, 1987; Ulerich, 1990) use qualitative models at this level of detail. With the development of formalisms for representing and reasoning with order of magnitude relations, fault simulation models that use more detailed information about the rough magnitude of parameters and relative size of variables have been developed (Dague et al., 1987). Order of magnitude formalisms have also been used for reasoning about the qualitative stability of stationary states in the startup of process plants (Aelion et al., 1992).

Various qualitative algebras for representing information at varying levels of detail have been developed in the last decade in the AI literature. The earliest and perhaps the most common is based on the algebra of signs called *confluences* (de Kleer & Brown, 1984). It consists of sign addition, subtraction, and qualitative equality. One of the main shortcomings of this algebra is the problem of ambiguity (Struss, 1990). A number of efforts have been made to strengthen sign algebras by introducing a finite set of landmarks (Forbes, 1984; Kuipers, 1987). However, a finite set of landmarks is not sufficient to overcome the ambiguity of addition and the lack of an additive inverse (Struss, 1990). Moreover, in real situations more detailed information, such as order of magnitude relations, is available and it is desirable to develop and use algebras that exploit this information. More recently, qualitative algebras that capture order of magnitude relations have been developed (Raiman, 1986; Mavrovouniotis & Stephanopoulos, 1987; Raiman, 1991; Dague, 1993a). The order of magnitude formalism O(M) provided by Mavrovouniotis & Stephanopoulos (1987) overcomes some of the shortcomings of the earlier approach (Raiman, 1986) and allows strict (mathematically sound) as well as heuristic interpretations for order of magnitude relations. However, the use of heuristic interpretation leads to invalid conclusions after the first inference step. Dague (1993b) has developed a formalism ROM(K) where each order of magnitude relation is represented by two overlapping intervals with different boundaries. This allows a formal treatment of the heuristic interpretation of order of magnitude relations and provides a sound calculus for multiple inference steps.

There is a growing effort in the AI literature to develop hybrid qualitative/quantitative algebras that allow the integration of numeric information into symbolic algebras (Dague, 1993b; Williams, 1991; Forbus & Falkenhainer, 1990; Berleant & Kuipers, 1990). In the AI literature, the information at different levels of resolution is preserved and the hybrid approaches are focussed on finding ways of scaling up and down these abstraction levels. The numeric information is generally used to resolve ambiguities that arise in qualitative algebras. An alternative approach to integrating qualitative and quantitative models involves transforming the qualitative relations into a quantitative framework and using numeric methods for reasoning with the integrated information. Raman and Grossman (1991) have developed such an approach for transforming qualitative knowledge expressed in propositional logic into algebraic constraints between integer variables that are then combined with other quantitative constraints between continuous variables in a mixed integer linear programming framework. Dague (1993b) has developed an approach for transforming order of magnitude relations into the real domain. In the real domain, the order of magnitude relations are expressed by intervals, and the bounds of the intervals are propagated using numeric consistency techniques (Lhomme, 1993). In this article, all of the order of magnitude information at various levels of resolution are converted into equality and inequality constraints between continuous variables. Subsequently, the order of magnitude relation between any pairs of variables is determined by solving for the minimum and maximum of the interval using a constrained nonlinear optimization approach. This optimization approach to order of magnitude reasoning is novel compared with the other approaches developed so far. We illustrate with examples that this approach provides more accurate results as compared to other approaches.

3. OPTIMIZATION APPROACH

The optimization approach consists of first transforming the order of magnitude relations into a set of algebraic constraints and then solving an optimization problem for inference. However, in order to describe this approach it is first necessary to choose a formal system that defines the syntax and the semantics for representing and reasoning with relative order of magnitude relations. The two main considerations for choosing a formalism are that it should provide an intuitive representation and should allow for sound and exact inferences. Two candidates are the O(M) formalism suggested by Mavrovouniotis and Stephanopoulos (1988) and the ROM(K) formalism suggested by Dague (1993a). For purposes of illustrating the optimization approach we have chosen the O(M) formalism. The strict interpretation of O(M) provides exact inferences, and we find that the O(M) relations are simpler and more intuitive as compared to the ROM(K) representation. However, the approach that we present here can be used with the ROM(K) formalism in a similar fashion. In this section we explicate how the O(M) relations can be transformed into algebraic constraints between continuous variables and provide an optimization formulation for inferring the order of magnitude relations between variables of interest.

The O(M) formalism proposed by Mavrovouniotis and Stephanopoulos (1988) is based on seven primitive relations between variables, which are shown in Table 1. Each relation is also described by a variable r_i, which is the ratio of the two variables X_1/X_2. The variable r_i is constrained to an interval based on the O(M) relation, for example, X_1 is much smaller than X_2 signifies the interval $(0, e)$ for r_1. Note that the O(M) relations relate absolute quantities without reference to their sign. Compound relations are represented by concatenating the primitive relations so that X_1 is less than X_2 is represented by $X_1 << \ldots -< X_2$, i.e., X_1 is much smaller to slightly smaller than X_2. There are in total 21 compound relations that can be represented by additional relations r_{ij}, $i = 1, \ldots, 7$, $j = i+1, \ldots, 7$. O(M) sanctions symmetry between variables and the intuition that for $X_1, X_2 > 0$, $X_1 - X_2 << X_2 \Leftrightarrow X_1 > X_2$. This leaves only one degree of freedom called the tolerance parameter e for defining the intervals for r_i. The intervals for r_i, $i = 1, \ldots, 7$ in terms of the parameter e are provided in Figure 1(a). In order to allow the inference $X_1 > X_3$ from $X_1 > X_2$, $X_2 > X_3$, a heuristic interpretation is adopted that replaces the nonoverlapping intervals in Figure 1(a) with overlapping intervals with fuzzy boundaries as shown in Figure 1(b). Both the relations (to the right and left) are valid in the fuzzy boundaries between intervals. In Table 2 we provide numerical values for the boundaries for different values of e. This tabulation is useful for the interpretation of the numerical results derived in examples.

We are now ready to formulate the optimization problem for reasoning about the relative orders of magnitude between two variables. For any two variables, if the order of magnitude relation is expressed as a primitive O(M) relation, then it can be transformed quite simply into an equality constraint using the ratio r_i, $i = 1, \ldots, 7$ with the upper and lower bounds on r_i specified as shown in Table 3. Similarly, any compound O(M) relation $X_1 r_{ij} X_2$ can also be written as an equality constraint $X_1/X_2 - r_{ij} = 0$, $i = 1, \ldots, 7$, $j = i+1, \ldots, 7$. However, the upper and lower bounds have to be determined as the lower bound of the smaller relationship, r_i, and the upper

Table 1. *Primitive relations of the O(M) formalism*

O(M) Relations	Verbal Explanation
$r_1 : X_1 << X_2$	X_1 is much smaller than X_2
$r_2 : X_1 -< X_2$	X_1 is moderately smaller than X_2
$r_3 : X_1 \sim< X_2$	X_1 is slightly smaller than X_2
$r_4 : X_1 == X_2$	X_1 is exactly equal to X_2
$r_5 : X_1 >\sim X_2$	X_1 is slightly larger than X_2
$r_6 : X_1 >- X_2$	X_1 is moderately larger than X_2
$r_7 : X_1 >> X_2$	X_1 is much larger than X_2

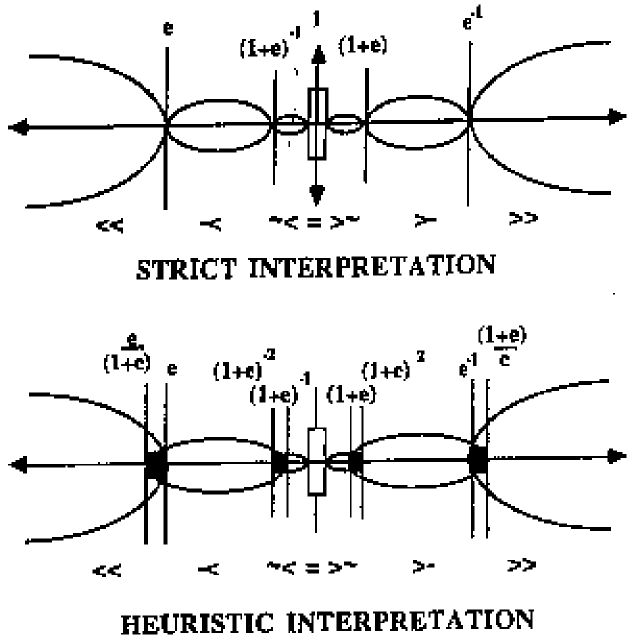

Fig. 1. Strict and heuristic interpretation of O(M) relations (Mavrovouniotis & Stephanopoulos, 1988).

Table 3. *Relational variables for optimization approach to O(M)*

O(M) Relation	Interval: Lower Bound, r_L	Interval: Upper Bound, r_U	Constraints
<<	0	e	$\frac{X_1}{X_2} - r_1 = 0$
−<	e	$\frac{1}{1+e}$	$\frac{X_1}{X_2} - r_2 = 0$
−<	$\frac{1}{1+e}$	1	$\frac{X_1}{X_2} - r_3 = 0$
==	1	1	$\frac{X_1}{X_2} - r_4 = 0$
>−	1	$1+e$	$\frac{X_1}{X_2} - r_5 = 0$
>−	$1+e$	$\frac{1}{e}$	$\frac{X_1}{X_2} - r_6 = 0$
>>	$\frac{1}{e}$	∞	$\frac{X_1}{X_2} - r_7 = 0$

bound of the larger relationship, r_j. This will become apparent as we solve examples in the next section. Alternatively, the compound relation r_{ij} can also be expressed as a pair of inequality constraints (as can the primitive relations) $r_i - X_1/X_2 \leq 0$, $X_1/X_2 - r_j \leq 0$, where the intervals for r_i and r_j are as shown in Table 3. This form is more convenient for automating the optimization formulation and has been used for implementation. Now, in order to derive the order of magnitude relation between any two variables Y_1, Y_2, their ratio ρ_k is expressed in an equality constraint $Y_1/Y_2 - \rho_k = 0$. The upper and lower bounds of the ratio ρ_k will determine the order of magnitude relation between the two variables. To obtain these bounds the following optimization problem is solved for maximum and minimum of the objective function Z_k:

Table 2. *O(M) boundaries*

e	0.05	0.1	0.2
$\frac{e}{1+e}$	0.0476	0.09091	0.1667
e	0.05	0.1	0.2
$\frac{1}{(1+e)^2}$	0.90703	0.82645	0.69444
$\frac{1}{1+e}$	0.95238	0.90909	0.833333
1	1	1	1
$1+e$	1.05	1.1	1.2
$(1+e)^2$	1.1025	1.21	1.44
$\frac{1}{e}$	20.0	10.0	5.0
$\frac{(1+e)}{e}$	21.0	11.0	6.0

$$\underset{\bar{X},\bar{r}}{\text{Optimize}} \quad Z_k = (\rho_k)^2,$$

where

$$\bar{X} = (X_1, X_2, \ldots, X_N)$$
$$\bar{r} = (r_1, r_2, \ldots, r_n)$$

subject to:

1. Constraints derived from the first principles, which describe the physics of the process:
$$h(\bar{X}) = 0$$
$$g(\bar{X}) \leq 0.$$
2. The relational constraints that describe the order of magnitude relations based on experiential knowledge:
$$h_r(\bar{X},\bar{r}) = 0$$
$$g_r(\bar{X},\bar{r}) \leq 0.$$

3. The bounds on the decision variables $\bar{X}, \bar{r}$. Note that the bounds for the variables $\bar{r}$ are based on a strict interpretation of the O(M) formalism shown in Table 3.

As stated earlier, since we want to relate the absolute magnitudes of quantities without bothering about their signs, both the maximization and minimization problems use the square of the ratio [of the two variables whose O(M) relation is desired] as the objective function. The solution of the series of maximum/minimum problems provides the upper/lower bounds for the ratios. Once the interval is determined, the order of magnitude relations based on the O(M) formalism [Figure 1(b)] can be derived. At this point one can use either the strict or the heuristic interpretation to determine the O(M) relation. However, if the results from this analysis are to be used for further analysis, then it is recommended that the intervals be used from a strict interpretation of O(M) since it preserves the soundness of the inferences for multiple steps.

4. EXAMPLES

In this section we provide three examples to illustrate the optimization approach for reasoning about order of magnitude relations. These examples involve solution of nonlinear algebraic equations. Hence, from the optimization perspective the problem is posed as a nonlinear programming (NLP) problem. The recent advances in NLP optimization techniques have provided several viable optimization algorithm options. The most popular of these are the generalized reduced gradient (GRG) and the successive quadratic programming (SQP) methods. Historically, the GRG strategy has been considered to be the less efficient mode of optimization (Biegler, 1983) for large-scale optimization problems. As a result, the SQP algorithm is used almost routinely for the solution of large-scale problems (Lang & Biegler, 1987). We have used the SQP algorithm for the solution of the examples provided below because this approach can then be easily extended to deal with large-size problems.

Amongst the three examples, the first example involves the analysis of a heat exchanger, and it illustrates how the optimization approach provides more accurate inferences as compared to conventional approaches. The second example compares the performance of a continuous stirred tank and a plug flow reactor, and illustrates the use of compound relations. Both of these examples are borrowed from Mavrovouniotis and Stephanopoulos (1988), where they used constraint satisfaction methods (assumption-based truth maintenance, ATMS) to solve for relative order of magnitude relations. This provides an opportunity to compare the results obtained from the optimization approach with the constraint satisfaction approaches. The third example deals with identifying qualitatively stable steady states in the context of process plant startup (Aelion et al., 1992) and illustrates the application of qualitative reasoning to control problems.

4.1. Heat exchanger

Figure 2 shows the schematic of a countercurrent heat exchanger. The important parameters for the heat exchanger simulation are also shown. The hot side input and output temperatures are T_{h1} and T_{h2}, respectively. Similarly, the T_{c2} and T_{c1} denote the cold side input and output stream temperatures, respectively. The temperature difference along the hot side is DTH and along the cold side it is DTC; these can be expressed as:

$$DTH = T_{h1} - T_{h2} \geq 0$$
$$DTC = T_{c1} - T_{c2} \geq 0. \quad (1)$$

The driving forces at the two ends of the heat exchangers are given by $DT1$ and $DT2$ and can be calculated using the following equations:

$$DT1 = T_{h1} - T_{c1} \geq 0$$
$$DT2 = T_{h2} - T_{c2} \geq 0. \quad (2)$$

From the definition of driving forces and temperature differences, the following equation results:

$$DTH - DT1 - DTC + DT2 = 0. \quad (3)$$

Considering the overall heat balance around the heat exchanger, where FH and FC denote the hot side and cold side molal flowrates, and KH and KC are the hot side and cold side molal heat capacities, respectively,

$$FH \times KH \times DTH = FC \times KC \times DTC. \quad (4)$$

Mavrovouniotis and Stephanopoulos (1988) assumed the following order of magnitude relations:

$$DT2 \;{-}{<}\; DT1$$
$$DT1 << DTH$$
$$KH \;{>}{-}\; KC. \quad (5)$$

From the order of magnitude relations and the constraints given above, they inferred five order of magnitude rela-

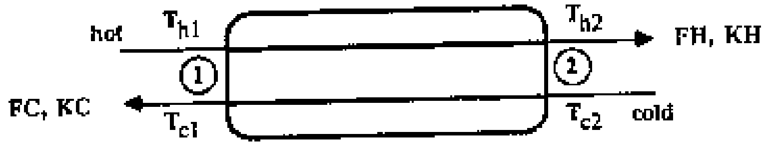

Fig. 2. Countercurrent heat exchanger.

tions involving $DT2$ and DTH, DTC and DTH, $DT1$ and DTC, $DT1$ and DTH, and FC and FH. In the following paragraphs we derive the order of magnitude relation between the same variables using the optimization approach.

Problem revisited using optimization approach

The optimization approach to O(M) involves formulation of the problem as minimization and maximization problems. The optimization approach for the heat exchanger problem is

$$\underset{\bar{X},\bar{r}}{\text{Minimize/Maximize}} \qquad Z_k = (\rho_k)^2,$$

where

$$\bar{X} = (TH1, TH2, TC1, TC2, DT1, DT2, DTH, DTC, FC, FH, KC, KH)$$

$$\rho_k \in \left(\frac{DT2}{DTM}, \frac{DTC}{DTH}, \frac{DT1}{DTC}, \frac{DT1}{DTH}, \frac{FC}{FH}\right)$$

$$\bar{r} = (r_1, r_2, r_3)$$

subject to:

1. Constraints derived from first principles that describe the physics of the process, Eqs. (1), (2), and (4).
2. The relational constraints that describe the order of magnitude relations (see Table 1 for definition of the ratio):

Table 4. *Interval identification for the heat exchanger*

O(M) Variables	e	Bounds	Interval Identification
$DT2$, DTH		$7.3015 \times 10^{-3} - 3.5704 \times 10^{-2}$	$4.7620 \times 10^{-2} > \frac{DT2}{DTH}$
DTC, DTH		$0.97754 - 0.99998$	$1 > \frac{DTC}{DTH} > 0.95238$
$DT1$, DTC	0.05	$3.0440 \times 10^{-[illegible]} - 3.0440 \times 10^{-2}$	$4.7620 \times 10^{-2} > \frac{DT1}{DTC}$
$DT1$, DTH		$2.9757 \times 10^{-4} - 4.7618 \times 10^{-2}$	$4.7620 \times 10^{-2} > \frac{DT1}{DTH}$
FC, FH		$1.04660 - 1.09975$	$1.10250 > \frac{DTC}{DTH} > 1$
$DT2$, DTH		$1.0940 \times 10^{-2} - 5.1088 \times 10^{-2}$	$9.0909 \times 10^{-2} \times \frac{DT2}{DTH}$
DTC, DTH		$0.96191 - 0.99999$	$1 > \frac{DTC}{DTH} > 0.90909$
$DT1$, DTC	0.10	$9.4757 \times 10^{-6} - 5.0972 \times 10^{-2}$	$0.09091 > \frac{DT1}{DTC}$
$DT1$, DTH		$4.9031 \times 10^{-2} - 9.0885 \times 10^{-2}$	$0.09091 > \frac{DT1}{DTH}$
FC, FH		$1.09120 - 1.19801$	$1.21000 > \frac{DTC}{DTH} > 1$
$DT2$, DTH		$2.0955 \times 10^{-2} - 1.1574 \times 10^{-1}$	$0.16667 > \frac{DT2}{DTH}$
DTC, DTH		$0.94072 - 0.99999$	$1 > \frac{DTC}{DTH} > 0.83333$
$DT1$, DTC	0.20	$8.5291 \times 10^{-2} - 1.9231 \times 10^{-1}$	$0.20000 > \frac{DT1}{DTC}$
$DT1$, DTH		$8.0235 \times 10^{-2} - 1.6667 \times 10^{-1}$	$0.16667 > \frac{DT1}{DTH}$
FC, FH		$1.16669 - 1.38462$	$1.44000 > \frac{DTC}{DTH} > 1$

$$\frac{DT2}{DT1} - r_2 = 0$$

$$\frac{DT1}{DTH} - r_1 = 0$$

$$\frac{KH}{KC} - r_5 = 0.$$

3. The bounds on the decision variables $\overline{X}, r$ (see Table 2 for upper and lower bounds for r):

$$0 \le \overline{X} \le 20000.$$

The above series of problems is solved for maximization and minimization of Z_k to obtain the upper and lower bounds for the relational ratios ρ_k. Since the relational constraints are expressed in terms of tolerance parameter e, the bounds are obtained for different values of e ranging from 0.05 to 0.2. The numerical results of the extremization are shown in Table 4. Using the boundary values for the heuristic interpretation provided in Table 2, we can derive the O(M) relations between the variables from the results of Table 4. It is interesting to note that as expected the O(M) relations do not depend on the value of e chosen for the interpretation of the O(M) relations.

Table 5 shows the O(M) interpretation of results for the case of e equal to 0.1. The last column of Table 5 presents the order of magnitude relations obtained by Mavrovouniotis and Stephanopoulos (1988) using ATMS. It can be easily seen from row 2 of Table 5 that O(M) does not infer that DTC is slightly less than DTH and therefore also fails to infer the relation between FC and FH correctly. On the other hand, the optimization approach infers all the order of magnitude relations correctly for all the tolerance parameters, in other words, DTH is slightly greater than DTC and FC is slightly greater than FH. This can be attributed to the fact that the optimization approach uses continuous representation of variables so no information is lost.

4.2. Comparison of continuous stirred tank reactor (CSTR) and plug flow reactor (PFR)

This example is also taken from Mavrovouniotis and Stephanopoulos (1988). In this example, compound O(M) relations are encountered that illustrate the formulation of inequality constraints for compound relations. The example demonstrates that the optimization approach successfully derives the unknown O(M) relations in the context of the two types of reactors CSTR and PFR and their comparison.

The example is centered around an irreversible first-order reaction, $A \Rightarrow B$ whose rate r is given by $r = k[A]$. The residence time of the reactor T in terms of volume of the reactor V and flowrate through the reactor F can be given by the following relation:

$$T = \frac{V}{F}. \tag{6}$$

And the time constant t of the reaction is specified as

$$t = \frac{1}{k}. \tag{7}$$

Assuming isothermal operation, the mass balance equations for each type of reactor can be expressed in terms of the concentration of reactant A in feed (C_1) and in the effluent (C_2). For a CSTR this leads to the following equation:

$$C_1 t - C_2 t - C_2 T = 0. \tag{8}$$

On the other hand, for the PFR reactor it results in

$$\ln\left(\frac{C_2}{C_1}\right) = \frac{T}{t}. \tag{9}$$

Mavrovouniotis and Stephanopoulos (1988) used a number of different O(M) relations between the residence time T and the reaction time constant t, as shown in Table 6, to derive the O(M) relations between the feed and

Table 5. *Relational interpretation for the heat exchanger*

O(M) Variables	Relational Interpretation	ATMS Results
$DT2, DTH$	$\frac{e}{1+e} > \frac{DT2}{DTH} \Rightarrow DT2 << DTH$	$DT2 << DTH$
DTC, DTH	$1 > \frac{DTC}{DTH} > (1+e)^{-1} \Rightarrow DTC -< DTH$	$DTC -<\ldots>- DTH$
$DT1, DTC$	$\frac{e}{1+e} > \frac{DT1}{DTC} \Rightarrow DT1 << DTC$	$DT1 << DTC$
$DT1, DTH$	$\frac{e}{1+e} > \frac{DT1}{DTH} \Rightarrow DT1 << DTH$	$DT1 << DTH$
FC, FH	$(1+e)^2 > \frac{DTC}{DTH} > 1 \Rightarrow FC >- FH$	$FC -<\ldots>- FH$

Table 6. *O(M) analysis of CSTR and PFR*

Given O(M) Relations	ATMS Results	
	CSTR	PFR
$T << t$	$C_2 -< C_1$	$C_2 -< C_1$
$T <\ldots> t$	$C_2 -< C_1$	$C_2 -< C_1$
$T >- t$	$C_2 -< C_1$	$C_2 <<\ldots -< C_1$
$T >> t$	$C_2 << C_1$	$C_2 << C_1$

Table 7. *O(M) relations and equivalent constraints for the optimization approach*

O(M) Relations	Equivalent Constraints
$T << t$	$\frac{T}{t} - r_1 = 0$
$T <\ldots> t$	$\frac{T}{t} - r_3 \leq 0$
	$r_2 - \frac{T}{t} \leq 0$
$T >- t$	$\frac{T}{t} - r_6 = 0$
$T >> t$	$\frac{T}{t} - r_7 = 0$

effluent concentrations (also shown in Table 6) for both PFR and CSTR. Their results were shown to capture the difference between the PFR and CSTR very well. In the next few paragraphs this problem is solved using the proposed optimization approach.

Problem revisited using optimization approach

The optimization approach for this problem involves solution of the following minimization and maximization problems for a number of different (given) O(M) relations between T and t, for both CSTR and PFR:

$$\underset{\bar{X},r}{\text{Minimize/Maximize}} \quad Z = (\rho_1)^2,$$

where

$$\bar{X} = (T, t, C_2, C_1)$$

$$\rho_1 = \frac{C_2}{C_1}$$

subject to the mass balance constraints given by Eq. (8) for CSTR and Eq. (9) for PFR. The different O(M) relations between the time constants given in Table 6 are converted in terms of the equality and inequality constraints shown in Table 7.

Table 8 provides the bounds derived for the ratio C_2/C_1 for various values of e. Using Table 2 we can verify that all of the O(M) relations derived using the optimization approach are the same as those derived by using ATMS. Table 8 also outlines the operating regions obtained using the optimization approach for tolerance parameter e equal to 0.1. This illustrates how the optimization approach also provides the operating regions over and above the qualitative relations.

4.3. Qualitative stability of stationary states

This example illustrates how the stability of stationary states encountered in the startup of process plants can be evaluated using qualitative information coupled with the optimization approach. Consider a chemical process subsystem that consists of a cooler and a reactor as shown in Figure 3. A typical scenario in the startup of process plants involves maintaining a low temperature reactor to prevent undesirable exothermic reactions between species A, B, which form the undesirable products U, with reaction rate $r_U = k[A][B]$. A proportional controller is used to keep the reactor temperature at or below a set point

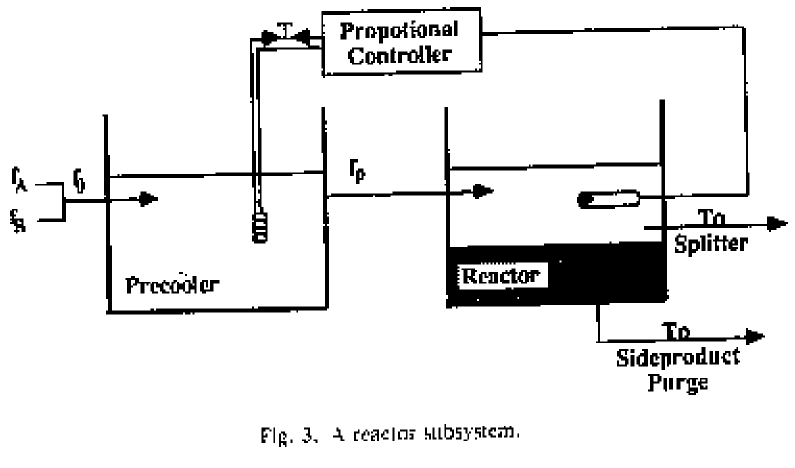

Fig. 3. A reactor subsystem.

Table 8. *Interval identification for the reactors,* C_1, C_2

T/t Relation	Bounds	Interval Identification
	CSTR	
$T << t$	$0.916645 - 0.949200$	$1 > C_2/C_1 > 0.90909$
$T <..> t$	$0.476167 - 0.50000$	$0.90909 > C_2/C_1 > 0.1$
$T >\sim t$	$9.098 \times 10^{-2} - 0.452489$	$0.90909 > C_2/C_1 > 0.09091$
$T >> t$	$1.994 \times 10^{-3} - 1.994 \times 10^{-1}$	$0.1 > C_2/C_1 > 0$
	PFR	
$T << t$	$0.91310 - 0.949200$	$1 > C_2/C_1 > 0.90909$
$T <..> t$	$0.332881 - 0.904841$	$> C_2/C_1 > 0.1$
$T >- t$	$8.941 \times 10^{-3} - 0.298236$	$0.90909 > C_2/C_1 > 0$
$T >> t$	$1.75 \times 10^{-2} - 1.75 \times 10^{-1}$	$0.1 > C_2/C_1 > 0$

T_{sp}. The coil can either add or remove heat. To avoid recycling hot material, the downstream valve to the splitter is closed. The primary concern is whether this subsystem can be started up to a stable steady state.

In order to evaluate the stability of this stationary state we write three energy balance equations for both the vessels and the temperature sensor as follows.

1. The energy balance for the precooler consists of heat removed by flow out through stream f_p, flow in through stream f_0, and the heat removed/added by the proportional controller:

$$m_p c_p \frac{dT_p}{dt} = f_0 c_p T_0 - f_p c_p T_p + K_c (T_{sp} - T_{ts}), \quad (10)$$

   where T_{ts} is the temperature measured by the sensor, and K_c is a proportional control constant.
2. The reactor energy balance consists of heat added by the flow stream f_p and the heat generated by the reaction:

$$m_r c_p \frac{dT_r}{dt} = f_p c_p T_p + X[A][B](-\Delta H_{rxn}) T_r, \quad (11)$$

   where the reaction rate constant has been replaced with its temperature dependence $k = XT_r$.
3. The sensor energy balance is based on the rate of heat transfer:

$$m_{ts} c_{p,ts} \frac{dT_{ts}}{dt} = hA(T_r - T_{ts}), \quad (12)$$

   where h is the heat transfer coefficient between the sensor and the reactor liquid, and $c_{p,ts}$, A are the heat capacity and area of the temperature sensor.

The key question that we are faced with is whether we can assure the stability of this system in the face of incomplete or qualitative information about the relative order of magnitude relations between various terms in the equations. In the following paragraphs we show how intuitive propositions stated in terms of order of magnitude relations can be formally verified using the optimization approach to O(M), and how we can derive order of magnitude relations that satisfy the stability requirements for stationary states.

Before we address these issues we reformulate Eqs. (10)–(12) in a matrix form and provide the Routh–Hurwitz conditions for stability. Equations (10)–(12) are linear and can be written in matrix form as follows:

$$\begin{bmatrix} \frac{dT_p}{dt} \\ \frac{dT_r}{dt} \\ \frac{dT_{ts}}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{f_p}{m_p} & 0 & -\frac{K_c}{m_p c_p} \\ \frac{f_p}{m_r} & \frac{M}{m_r c_p} & 0 \\ 0 & \frac{hA}{m_{ts} c_{p,ts}} & -\frac{hA}{m_{ts} c_{p,ts}} \end{bmatrix} \begin{bmatrix} K_c T_{sp} \\ 0 \\ 0 \end{bmatrix}. \quad (13)$$

Denoting the elements of the matrix by the shorthand notation a_{ij}, $i, j = 1, \ldots, 3$, we can write the Routh–Hurwitz conditions as follows:

$$k_1 = a_{11} + a_{33} - a_{22} > 0 \quad (14)$$

$$k_2 = a_{11} a_{33} - a_{11} a_{22} - a_{22} a_{33} > 0 \quad (15)$$

$$k_3 = a_{13} a_{21} a_{32} - a_{11} a_{22} a_{33} > 0 \quad (16)$$

$$\begin{aligned} \delta_2 = &(a_{11}^2 a_{33} + a_{11} a_{33}^2 + a_{11} a_{22}^2 + a_{22} a_{33}^2) \\ &- (a_{11}^2 a_{22} + 3 a_{11} a_{22} a_{33} + a_{22} a_{33}^2) > 0 \end{aligned} \quad (17)$$

$$\delta_3 = k_3 \delta_2 > 0. \quad (18)$$

The Routh–Hurwitz conditions are not stringent criteria in that they do not restrict the parameters to single values but rather define a domain of stability in the parameter space. This provides a basis for using qualitative specifications to ascertain stability.

Hypothesis testing using optimization approach to O(M)

It is clear from the matrix in Eq. (13) that the term a_{22} which represents the exothermic reaction is a positive feedback which could render the system unstable. Intuitively, it appears that if the exothermic reaction term is much smaller than other diagonal gain terms, then the system should stabilize. We will now illustrate how this intuition can be cast in an O(M) formalism and then use the optimization approach to verify this hypothesis.

To test this hypothesis one needs to find the relation between the diagonal terms a_{11}, a_{33} and the exothermic reaction term a_{22}. The optimization problems can be formulated as

$$\underset{\bar{X},\bar{r}}{\text{Minimize/Maximize}} \qquad Z_k = (\rho_k)^2,$$

where

$$\bar{X} = (a_{11}, a_{13}, a_{21}, a_{22}, a_{32}, a_{31})$$

$$\rho_k = \left(\frac{a_{11}}{a_{22}}, \frac{a_{33}}{a_{22}}\right)$$

$$\bar{r} = (\phi)$$

subject to the five constraints [Eqs. (14)-(18)] for stability considerations and the following approximate bounds on the parameters:

$$0.01 \le \bar{X} \le 100.$$

The lower bounds of both ρ_1 and ρ_2 are found to be smaller than $e/1 + e$ and the upper bounds smaller than 1 where the range of tolerance parameter e varied from 0.05 to 0.2. This result confirms the hypothesis that the conditions $a_{22} << a_{11}$ and $a_{22} << a_{33}$, in other words, the heat of reaction term is much much smaller than the other diagonal gains, is sufficient for stability. The interesting result however is that the optimization approach provides a much less restrictive sufficiency condition for stability, in other words, $a_{22} < a_{11}$ and $a_{22} < a_{33}$. These O(M) relations are derived from the bounds derived for the ratios and shown in Table 9.

5. DISCUSSION

Mavrovouniotis & Stephanopoulos (1988) have outlined the hierarchy of models encountered in engineering systems according to their level of abstractions. This hierarchy consists of:

- Boolean models that identify the existence or nonexistence of constraints among parameters.
- Qualitative models represent the next level of abstraction and include signs of the variables and direction of their effect along with the existence and nonexistence of constraints.
- Order of magnitude models also have information about relative orders of magnitudes of the quantities.
- Quantitative models involve the most detailed numerical and algebraic representations.

The use of quantitative models dominates the practice of engineering and science. Sophisticated quantitative modeling platforms, and large-scale modeling simulators based on numerical and algebraic solution techniques, are widely available. However, for most problems a fair amount of qualitative knowledge at different levels of the above hierarchy is available in addition to the quantitative models. However, most quantitative modeling platforms and simulators are unable to use this qualitative information. A unified framework that can incorporate information at all levels of the above hierarchy into its inference would be desirable. Furthermore, given the availability of the powerful numerical techniques, it would be most useful if qualitative information at various levels can be used within the same numerical framework as the quantitative models. In this article we have illustrated how this can be achieved.

We present an approach where one can use the order of magnitude knowledge in the same numerical framework as that of quantitative models. The O(M) relations are converted into linear and nonlinear constraints that can be easily coupled with the quantitative models also expressed as linear and nonlinear constraints. The problem is phrased as a nonlinear programming (NLP) optimization problem. The qualitative models that are at the next level in the hierarchy can also be similarly represented by nonlinear equality and inequality constraints. For example, the signs of variables such as X_1 is positive can be expressed as an inequality constraint given by $X_1 > 0$. So, it is possible to incorporate this qualitative knowledge in the NLP framework described above. Boolean models, on the other hand, cannot be incorporated into the NLP framework since discrete decisions variables are encountered. However, these logic variables representing discrete decisions can be expressed mathematically as integer binary variables, and reasoning is equivalent to solving a mixed-integer linear programming (MILP) model. Therefore it is apparent that the optimization approach involving solutions of mixed-integer nonlinear programming (MINLP) models could encompass the complete modeling hierarchy and will lead to the unified modeling platform that we are looking for.

Table 9. *Interval identification for the steady states, $e = 0.1$*

O(M) Variables	Bounds	Interval Identification
a_{11}, a_{22}	$1.00 \times 10^{-3} - 0.99$	$1 > a_{22}/a_{11} > 0$
a_{33}, a_{22}	$1.00 \times 10^{-3} - 0.99$	$1 > a_{22}/a_{11} > 0$

6. CONCLUSIONS

We have provided a methodological approach for transforming order of magnitude relations into a numerical framework, and the use of nonlinear optimization techniques for inferring order of magnitude relations. We have illustrated this approach with examples from the AI literature and shown that the optimization approach provides more precise order of magnitude relations as compared to conventional constraint satisfaction approaches. This provides a crucial step in developing unified frameworks that allow the incorporation of qualitative information at various levels of abstractions into numerical frameworks used for reasoning with quantitative models. This has far-reaching implications regarding the simplicity with which large-scale simulators used in engineering can be augmented to incorporate qualitative models.

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