

A Stochastic Approach to Qualitative Simulation using Markov Processes

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Abstract

Interval based value representation methods constitute a major technical foundation of qualitative reasoning, but they necessarily generate ambiguous situations and spurious solutions. Ambiguity may be reduced by introducing more information and knowledge: either in the form of supplementary quantitative information or by applying general rules, taken from systems theory, on the behavior of dynamic systems. In the second approach concepts as state space diagrams or qualitative cells are exploited. The set of solutions is reduced and general classes of behavior are described. But the concrete behavior still depends on known information, and still too many things cannot be excluded. The application of stochastic concepts could exploit a further type of knowledge: some vague information in the form of priorities or the strength of some influence. The concept of Markov processes provides a similar description as the state space approach, but indicates priorities of different behaviors in solution space as well. This paper demonstrates how existing approaches in qualitative simulation can be transformed appropriately.

1 Introduction

Interval based value representation methods constitute a major technical foundation of qualitative reasoning, but they necessarily generate ambiguous situations and spurious solutions [Struss, 1987; Kuipers, 1985; Kuipers, 1986]. Ambiguity may be reduced by introducing more information and knowledge: either in the form of supplementary quantitative information [Kuipers and Chiu, 1987; Kuipers and Berleant, 1988; Berleant, 1989; Berleant and Kuipers, 1990] or by applying general rules on the behavior of dynamic systems [Lee and Kuipers, 1988; Kuipers *et al.*, 1991; Struss, 1988]. Since qualitative reasoning deals with dynamic systems, similar to systems theory, concepts of the latter field can be applied. The works of [Sacks, 1990a; Sacks, 1990b; Ishida, 1989; Ishida, 1992; Aubin, 1992] which exploit state space diagrams, the course of trajectories or the concept of qualitative cells justify this correspondence. These approaches describe the

entire space of solutions and, by applying general rules, are able to exclude further spurious solutions. The set of solutions is reduced. And they can define general classes of behavior. But the concrete behavior still depends on known information, such as initial or parameter values. The application of stochastic concepts could exploit a further type of knowledge: some vague information in the form of priorities, a degree of possibility or a strength of some influence. The concept of Markov processes [Freedmann, 1971] provides a similar description as the state space approach, but indicates priorities of the different behaviors in that space as well. Assuming the existence of such vague information this approach may deliver more information.

The structure of the paper is the following one: the next chapter describes a constructive approach in qualitative simulation, based on a fuzzy representation of values. This will serve as a prototypical example to apply the concept of Markov processes, which are briefly explained in chapter 3. The subsequent chapter demonstrates the use of this method and shows its benefits. In the concluding remarks both the advantages and restrictions of this approach as well as directions of further work are emphasized.

2 QUALSIM - an Approach Using Fuzzy Sets

Based on crisp intervals a qualitative value can only lie in one specific range. But sometimes even this knowledge is not available. A value might fall in some region, or not, more than one assignment is possible. This kind of knowledge can often be found in modelling when experts in the respective field apply simulation and modelling methods to new phenomena [Guariso *et al.*, 1992]. It has to do with beliefs that exist relative to assumptions about the modelled reality. It is different from the concept of probability which just deals with exclusive cases, here the possibility of being in two ranges at the same moment may be higher than one. Fuzzy sets are a means to implement and compile such knowledge, and furthermore, this approach may also supply methods for calculation [Yager *et al.*, 1987]. It possesses a double relationship to crisp interval based methods: on one side it deals with situations where exact ranges are not exactly known and on the other

side the result of the reasoning process may denote priorities on the different possible behaviors as well.

QUALSIM, based on fuzzy sets, may serve as an example to demonstrate the feasibility of the proposed approach. QUALSIM [Guariso *et al.*, 1989; Guariso *et al.*, 1992] is based on influence diagrams. Causality is identified in the modelling process and compiled into the model. The algorithm can be seen as a constructive one, dedicated to the straightforward generation of a qualitative behavior of a system. In close relationship to numerical simulation time is considered as an integer counter, a unit increment corresponding to a computation step. This may or may not indicate a change of the system's state.

The value of a state variable may take one of the following labels from the set Q of qualitative values:

+/- EXTRALARGE
+/- LARGE
+/- MEDIUM
+/- SMALL
+/- EXTRASMALL
ZERO

QUALSIM assumes that the entire range of possible values of a variable can be defined in advance. This representation covers the whole range, it is finite, ordered and associative excluding the extreme intervals on both sides. But this is no hard restriction since the knowledge of the entire range is assumed to exist. Thus, each variable x is identified by a numeric range R_x defined as a subrange of the real number space. Each value of the magnitude is a fuzzy set defined by delimiting values v_k , $k = 1, \dots, 12$ (by default the v_k 's are evenly spaced in the positive and negative subintervals of R) and a tuple (v_k, a, b) defining a fuzzy membership function $\mu_A(x)$ (similar to [Shen and Leitch, 1990; Shen and Leitch, 1991] and different to the original notion of QUALSIM):

$$\mu_A(x) = \begin{cases} 0 & x < v_k - a \\ \frac{x - v_k + a}{d + a} & x \in [v_k - a, v_k + d] \\ 1 & x \in [v_k + d, v_{k+1} - d] \\ \frac{v_{k+1} + b - x}{d + b} & x \in [v_{k+1} - d, v_{k+1} + b] \\ 0 & x > v_{k+1} + b \end{cases}$$

for each k and the corresponding $A \in Q$. In the case of the two delimiting points v_1 and v_{12} $\mu_A(x)$ remains at a value of 1.

The constant d is defined global and determines, together with the variable dependent values a and b , the fuzziness of the qualitative values.

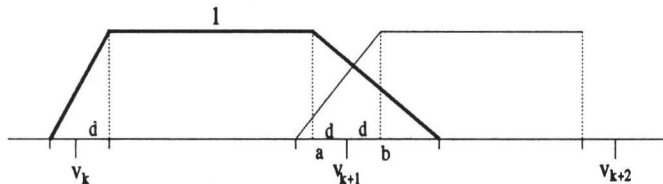


Figure 1: Fuzzy set based value representation

Connections between two variables may possess one of the following labels:

+/- EXTRASTRONG
+/- STRONG
+/- MEDIUM
+/- WEAK
+/- EXTRAWEAK

These labels are assumed to correspond to numeric subranges of the interval $[-1, 1]$. They are instantiated to specific numeric values c_{ij}^0 randomly distributed in the respective subrange. The probability distribution of these values is normal and centered on the center of the subrange. Standard deviation σ_{ij} is chosen by the user in order to reflect his/her subjective perception of the uncertainty of the connection. For instance, if the user selects the default value $\sigma_{ij}=0$, the distribution is reduced to an impulse and represents a high confidence in the appropriateness of the selected value. For simplicity, in the following we will only consider this case. Thus a kind of an influence graph is constructed [Scheines *et al.*, 1991] (see figure 2), indicating the strength of a connection and not its probability (as in [Wellman, 1988; Pearl, 1986; Peot and Shachter, 1991]).

The algorithm is based fundamentally on the conversion of qualitative values into quantitative ones and vice versa. The propagation of the uncertainty during the simulation is represented by the bifurcation of the simulation tree.

- At the beginning of the simulation the initial qualitative value for state variable x is transformed into its numeric equivalent x^0 being the characteristic point of the relative fuzzy set (i.e. its center).
- Given a qualitative value $x_i(t)$ and numeric value $x_i^0(t)$ for the state variable at time t and assuming that $I_i = \{x_j : x_j \text{ is connected to } x_i, j \in 1..n\}$ is the set of variables that exert an influence on the variable x_i , the new numeric value is computed as

$$x_i^0(t+1) = x_i^0(t) + \sum_{j \in I_i} \Delta x_j(t)$$

$$\text{where } \Delta x_j(t) = c_{ji}^0 \frac{x_j^0(t)}{R_{x_j}} R_{x_i}$$

and c_{ij}^0 is the mean value of the connection between x_i and x_j and R_x is the range of the respective variable.

- Since QUALSIM distinguishes between state and output variables, the latter ones are calculated similarly to state variables. It follows that the influencing arcs of QUALSIM represent either an integration step (when state variables are influenced) or in the case of output variables just an influence. Given a qualitative value $y_i(t)$ and its numeric value $y_i^0(t)$ for the output variable at time t , assuming again that $K_i = \{x_j : x_j \text{ is connected to } y_i, j \in 1..n\}$ is the set of variables that exert an influence on y_i , the new numeric value is computed as

$$y_i^0(t+1) = \sum_{j \in K_i} \Delta x_j(t) \text{ and } \Delta x_j \text{ is calculated as before.}$$

being random variables and S the finite set of states then a Markov chain is a sequence of the random numbers where $P[X_n = s_j | X_1, \dots, X_{n-1}] = P[X_n = s_j | X_{n-1}]$. Homogeneous Markov chains do not depend on n , i.e. $p_{ij} = P[X_n = s_j | X_{n-1} = s_i]$ does not depend on n (p_{ij} is independent from time; see [Freedman, 1971; Pflug, 1986]). This is the probability that the system changes from state s_i to state s_j . These probabilities can be written in the form of a quadratic matrix P indicating the state transition probabilities for all combinations of states. The rows of this matrix sum up to 1, i.e. a state has to change to its successors. The initial situation can be described by a row vector v , i.e. v is a probability distribution describing the probability of each state being initial state. Multiplying v with P gives a vector w , i.e. $w = v * P$, which describes the probability of the system being in a specific state after the first transition, at the second time point. In a stationary case $v = w$, the probabilities are not changed by applying P . Matrix P describes the transition probabilities in one step, multiplying P with P , the transition table is generated for two steps. Thus, P^n describes the transition probabilities of applying n transitions, i.e. the situation of the system after n steps.

Matrix P has some nice properties, for example it classifies the states into equivalence classes. A state s_j may be reached from s_i if $\exists n$ and $n > 0$, that $p_{ij}^n > 0$ (written as $s_i \rightarrow s_j$; this is no logical implication!), otherwise it cannot be reached from s_i . If both $s_i \rightarrow s_j$ and $s_j \rightarrow s_i$ are valid, then s_i and s_j are called equivalent ($s_i \leftrightarrow s_j$). Those states which are equivalent to each other form an equivalence class. If the system has left an equivalence class once, it can never return. Such classes are partially ordered by the following definition: G_1 is before G_2 if $\exists s_i \in G_1$ and $\exists s_j \in G_2$ and $s_i \rightarrow s_j$. Thus, not only probabilities for specific behaviors may be derived from a transition matrix, but the sequence of visited states or the existence of cycles can be indicated as well.

4 Markov Processes in Qualitative Simulation

The application of this method to the QUALSIM approach requires the consideration of some problems:

- the fuzzy number representation of QUALSIM has to be converted to a probabilistic form to guarantee some Markov properties,
- QUALSIM denotes the strength of an influence between variables, no state description is given in advance,
- the entire set of possible system states is not known.

The solution of the first point makes a "normalized" representation of the qualitative values necessary, i.e. $\sum_{A \in Q} \mu_A(x) = 1$ for every $x \in R_x$, i.e. fuzzy numbers are transformed in order to represent probabilities.

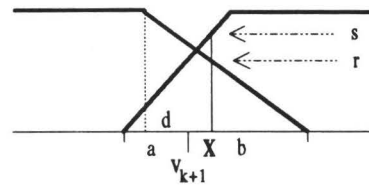


Figure 3: Relationship between two fuzzy numbers

Such a transformation has to maintain the relationship between the two fuzzy numbers, i.e. if x is the current value of the respective state variable the following has to be satisfied:

$$r:s = \frac{b-x}{d+b} : \frac{a+x}{d+a} \text{ and } r+s=1.$$

The important feature is the relationship between both values and not their magnitudes.

The second and the third problem can be discussed together: The set of system's state S can be constructed in advance based on the limited value set of the qualitative quantity space. If $w = \#(W)$ denotes the number of state variables (W is the set of state variables) and $u = \#(Q)$ the number of qualitative values, then the number of all possible states is u^w . Therefore, the set S can be generated by enumerating all possible value combinations for each element of W . Each element of S is a vector, the first member of the vector representing the value of the first variable, the second member representing the value for the second state variable, and so on. Every value combination represents a state and for every combination of values the respective state can be identified. Thus, the finite state space is constructed.

$\text{succ}(m | m \in Q)$ denotes the neighbour which follows a member of Q , and $\text{pred}(m | m \in Q)$ the neighbour which precedes a member of Q . LARGE is $\text{succ}(\text{MEDIUM})$ and SMALL is $\text{pred}(\text{MEDIUM})$. $\text{succ}(\text{EXTRALARGE})$ is defined to be EXTRALARGE, $\text{pred}(-\text{EXTRALARGE})$ is -EXTRALARGE again. The transition probabilities $P_{S_i S_j}$, i.e. going from state S_i to state S_j can now be derived (S_{ik} denotes the k^{th} component of vector S_i - with $S_{ik} \in Q$ - and G denotes the distribution of the numerical correspondents R_{ik} of a qualitative value S_{ik}):³

$$P_{S_i S_j} = \begin{cases} 0 & \text{if } S_{jk} \notin \{\text{pred}(S_{ik}), S_{ik}, \text{succ}(S_{ik})\} \\ \int \mu_{(S_{jk})}(\sum_q R_{iq} \times c_{qk} + R_{ik}) dG & \text{otherwise} \end{cases}$$

The probability to change from S_i to S_j - the system is in S_i at time t and in S_j at time $t+1$ - is zero when the law of continuity is violated. R_{iq} correspond to those components q (i.e. state variables) that influence the state variable k of W . The second part represents the original formula to calculate the new value of a state variable where the quantitative correspondent of a qualitative value is weighted by the respective probability distribution. Based

³ G can be obtained by applying the model equations to produce the trajectory of the system. Depending on the c_{ij} this trajectory takes only a finite number of quantitative values inside each qualitative range. Each of these points has thus a well defined probability of occurrence.

on the fact that variables vary continuously, it follows that P is very sparse. Every state S_i may just have 3^w successors since in each transition just three possibilities of change for each state variable exist, i.e. in each row of P a small number of elements is $\neq 0$.

Since $p_{S_i S_j k}$ represents just the k^{th} component of a vector of probabilities several approaches can be applied to approximate the overall probability to go from S_i to S_j .

a) Since the decisions of choosing a specific range for each component of a state variable are independent, in cases where the state variables are only loosely coupled the multiplication of the single components of the probability vector is a reasonable operation, i.e. $p_{S_i S_j} = \prod_k p_{ijk}$. Rewriting $p_{S_i S_j}$ as p_{ij} , the Markov property of $\sum_{j \in \text{succ}(S_i)} p_{ij} = 1$ can be demonstrated as described in the following.

The single p_{ijk} elements can be grouped as a matrix with dimension $w \times 3^w$, w is the number of state variables:

	S_1	S_2	S_3	S_{3^w}
S_i	p_{i11}	p_{i21}	p_{i31}	p_{i3^w1}
	p_{i12}	$:$	$:$	$:$
	$:$	$:$	$:$	$:$
	p_{i1w}	p_{i2w}	$:$	$p_{i3^w w}$

The formula $\sum_{j=1}^{3^w} \prod_{k=1}^w p_{ijk} = 1$ can be shown by induction:

If $w = 1$ then S_i has just 3 successors S_j which depend on the value of S_i , either $\text{pred}(S_i)$ or S_i or $\text{succ}(S_i)$. Given the initial normalisation of the membership functions these three probabilities sum up to 1.

Now, assuming that the above formula is true for the number of state variables being n , it can be shown that it holds for the number being $n+1$ as well. The respective matrix is obtained by adding one row for the probabilities of state variable $n+1$ which triples the number of columns:

$p_{i1n+1} :$	p_{i1n+1}	$p_{i2n+1} :$	p_{i2n+1}	$p_{i3n+1} :$	p_{i3n+1}
$p_{i11} :$	p_{i3^n1}	$p_{i11} :$	p_{i3^n1}	$p_{i11} :$	p_{i3^n1}
$p_{i12} :$	$:$	$p_{i12} :$	$:$	$p_{i12} :$	$:$
$:$	$:$	$:$	$:$	$:$	$:$
$p_{i1n} :$	$p_{i3^n n}$	$p_{i1n} :$	$p_{i3^n n}$	$p_{i1n} :$	$p_{i3^n n}$

p_{i1n+1} is the probability that variable $n+1$ does not change its value at the next state, p_{i2n+1} that the next value is $\text{succ}(S_{in+1})$, p_{i3n+1} that the next value is $\text{pred}(S_{in+1})$. The sum of these three sum up to 1. By

$$1 = p_{i1n+1} \times 1 + p_{i2n+1} \times 1 + p_{i3n+1} \times 1 =$$

$$= p_{i1n+1} \times \sum_{j=1}^{3^n} \prod_{k=1}^n p_{ijk} + p_{i2n+1} \times \sum_{j=1}^{3^n} \prod_{k=1}^n p_{ijk} + p_{i3n+1} \times \sum_{j=1}^{3^n} \prod_{k=1}^n p_{ijk} =$$

and by modifying the indices, for example $p_{i1n+1} = p_{i1n+1}$, and by changing the order of summation and multiplication

$$= 3 \times \sum_{j=1}^{3^n} \prod_{k=1}^{n+1} p_{ijk} = \sum_{j=1}^{3^{n+1}} \prod_{k=1}^{n+1} p_{ijk}, \text{ the formula is true for}$$

$w = n+1$. Thus the Markov property is satisfied.

b) Instead of multiplying the components of the probability vector, the minimum of the components could

be chosen. This would mean that the most unlikely case inside each column determines the overall probability of this specific transition. The inertest variable determines the behavior of the system. In this case a strong dependence between the state variables is assumed. To obtain the Markov property every single value has to be weighted by the row sum of all minima, i.e.

$$p_{ij} = \frac{\min_k (p_{ijk} | k \in 1..w)}{\sum_j \min_k (p_{ijk} | k \in 1..w)}.$$

c) As a final approach the single components of each vector could be added. Also in this case we assume a strong dependence between the model's variables. A possible interpretation would be some kind of averaging the transition probabilities which of course makes only sense if no component has a probability of zero. In this approach the value can be calculated by the following formula $p_{ij} = 1/F_w \times \sum_k p_{ijk}$.

The factor F_w represents the sum over all components of p_{ij} for all successor states S_j of S_i , i.e. $\sum_k \sum_{j \in \text{succ}(S_i)} p_{ijk} = F_w$, where F_w is defined recursively: $F_0=0$ and $F_i=3 \times F_{i-1} + 3^{i-1}$, $\forall i > 0$. This can be easily proved by induction similar to the case of multiplication. Now the row sum of P is 1, satisfying the Markov property of $\sum_j p_{ij} = 1$.

5 Conclusions

The choice of the method to compute the single probability still has to be explored. It can be assumed that the concept of reachability and velocity of reaching specific states will depend on this choice. And it has to be confronted with the simulation results of the original approach.

The matrix P represents the state space of the system and the simulation of a system is now done by multiplications of matrices and vectors, describing the initial state of the system. These are simple operations, but the dimension of the matrix - even if it is very sparse - may be enormous. However, it can be built in advance and provides a description of the state space indicating privileged behaviors. Moreover, it can be used to divide the state space into equivalence classes, giving a qualitative interpretation of the whole state space. This work shows that, given uncertain information in the form of possibilities or probabilities, this information can be used by the means of Markov processes to generate the entire set of solutions, denoting priorities among them as well.

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