# MARK - A Simulation System for Parameter Estimation in Simulation of Ecological Processes

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#### Abstract

In this work I present a Prolog program MARK, I developed, for parameter estimation in the simulation of ecological systems, capable of qualitatively explaining the simulated system. To generate qualitative explanation, the program combines a numerical and a qualitative simulator. The program was tested on a number of simple ecological models. The work is motivated also by educational needs: such "explanatory simulations" are better suited for tutorial purposes than the traditional purely numerical simulations.

#### 1. Introduction

Jørgensen [5] introduces a crucial problem for this work - the estimation of system parameters in simulation, which could guide the process toward desired behaviour. Jørgensen presents a large space of interesting ecologic dynamic systems, thus providing an initial motivating framework for the research.

The QSIM algorithm [6] is usually used for qualitative simulation based on QDE and gives symbolic description of system behaviour. That is the reason why such simulation is a more suitable basis for explanation generation than common numerical simulation. At the same time Kuipers' algorithm has known disadvantage, generating besides real also fictious behaviours. This work is an effort also towards solution or at least diminution of the mentioned problem.

One important problem is the need for intelligent tutoring systems and learning environments for education and training [4] - such a simulation system named MARK is developed (figure 1).





# 2. Qualitative analysis of ecological systems by "intelligent" numerical simulation

"Intelligent" numerical simulation algorithm is based on the following hypothesis for system described by system of n ODE and for m coefficients.

Hypothesis: QualitativeBehaviour(k<sub>1</sub>, k<sub>2</sub>, ..., k<sub>m</sub>) = QualitativeBehaviour(k<sub>1</sub>+ $\Delta$ , k<sub>2</sub>, ..., k<sub>m</sub>)  $\Rightarrow \forall \epsilon$ , 0<= $\epsilon$ <= $\Delta$ , QualitativeBehaviour(k<sub>1</sub>+ $\epsilon$ , k<sub>2</sub>, ..., k<sub>m</sub>) = QualitativeBehaviour(k<sub>1</sub>, k<sub>2</sub>, ..., k<sub>m</sub>)

#### This is interpreted as:

If two behaviours are qualitatively equal for two coefficient value combinations, where one coefficient has its values at the bounds of interval Delta, keeping at the same time all other coefficient constant, then all behaviours obtained by changing the varying coefficient are qualitatively equal to those at bounds of Delta, for every step Epsilon with given properties. (figure 2)

The hypothesis is tested for every coefficient, in order to observe hypothesis "probability" in dependence of interval Delta, which is decreasing by bisection.



Figure 2: Testing hypothesis for coefficient k1

Corresponding "probability" for each Delta, obtained for small enough step Epsilon, is expressed as the proportion of the number of qualitatively equal behaviours (EqualB) and the number of the qualitatively different behaviours (DiffB), in comparison to those at Delta bounds. Conclusions about coefficient sensitivity are made, using the data from the hypothesis test results. The goal is to find DeltaMin (and respective Epsilon), whose proportion DiffB/EqualB is small enough to satisfy the hypothesis condition.

Hypothesis test shows (for an ecosystem with feedback whose conceptual diagram is given in figure 3) that it is sufficient for coefficient k4 to choose Delta=0.000999 (table 1), to obtain constant behaviour on Delta for Epsilon defined as in hypothesis. In the case of coefficients k1, k2 and k3 further sensitive analysis is desirable, so the DeltaMin - bisection condition limit should be decreased (also respective small step Epsilon).

So, having at points A, B, C and D (figure 2) qualitatively equal behaviours, and (k12-k11) and (k22-k21) less than corresponding satisfactory Delta values from hypothesis test, the conclusion could be made that at all points inside marked rectangle behaviours are qualitatively equal, keeping the coefficient other than k1 and k2 constant. In this way it is possible to analyse a given system through discovering all possible qualitatively different behaviours. However, this method is limited by the restricting bisection condition (the size of minimum Delta - DeltaMin), by the size of small step Epsilon, and by the computational complexity of the algorithm.

Coefficient	Delta	Worst	Average
		W	value A
k1	0.000999	13.0	13.0
	0.0004995	6.0	4.25
	0.0002497 5	all_different	all_different
k2	0.0999	0.4	0.4
	0.04995	0.75	0.375
	0.024975	2.0	0.5
k3	0.000999	0.272	0.272
	0.0004995	0.75	0.375
	0.0002497 5	2.0	0.625
k4	0.000999	0.0	0.0

**Table 1:** Hypothesis validation depending on  $\Delta$ , for an ecosystem with feedback



Figure 3: Conceptual diagram of an ecosystem with feedback

# 3. Qualitative simulation

Kuipers [6] describes a qualitative simulation algorithm QSIM, which is guaranteed to predict all real behaviours of system consistent with the model. However, the QSIM algorithm may not be sufficiently powerful to filter out all inconsistent spurious behaviours. This work is an effort also towards solution or at least diminution of the mentioned problem, using the "intelligent" numerical simulation algorithm. The version of the Prolog program SI2LOGIC, based on the QSIM kernel qualitative simulation algorithm, which is used by MARK, was programmed by Alen Var{ek and modified by prof. Ivan Bratko [2].

# 3.1. An implementation of the "intelligent" numerical simulation algorithm improving QSIM predicting method and parameter estimation in simulation

"Intelligent" sampling algorithm is used to search for at least one coefficient combination for every qualitative behaviour QSIM has predicted. It is desirable that algorithm marks all real behaviour tree branches. (figures 4 and 5). In that way the algorithm improves QSIM behaviour predicting method.

Marking the QSIM qualitative behaviour tree for given QDE model and initial state, has reduced the behaviour tree. Only really possible behaviours are retained. These are marked by a corresponding combination of parameter values. As a test model an ecosystem with feedback has been used, and the results are given in table 2. For each tree level the value in first column represents the number of total system states predicted by QSIM and the value in the second column represents marked system states at that level. Because of computational complexity, test is completed only for Depth=3.

In order to obtain more precise results (not to skip real behaviours), coefficient values are varied in small enough steps, dependent on coefficient sensitivity (obtained earlier by hypothesis test). Because of computational complexity and overflow problems coefficients change their value in rather narrow intervals.

Experts could benefit from marked tree noticing rules that govern the relationships between the coefficients. In that way they could extend their ecological knowledge. If this is the aim of study, changing of coefficient values can be adapted to observe the relationships of interest.



Figure 4: Marking the QSIM qualitative tree



Figure	5:	Marked	QSIM	behaviour	tree
	•••		~~~		

Tree	Number of system	Number of system	
level	states predicted by	states marked as	
	QSIM	real	
0	1	1	
1	1	1	
2	1	1	
3	2	1	

Table 2: Real and spurious states at tree levels for an ecosystem with feedback

## 4. Generating behaviour explanations

MARK generates following explanation for the behaviour of the prey biomass in the "predatorprey" ecological model (figure 6). Conclusion about behaviour periodicity is made:

Prey biomass is between 0 and a0 decreasing, is between 0 and a0 reaching local minimum, is between 0 and infinity increasing, is between a0 and infinity reaching local maximum, is between a0 and infinity decreasing. Behaviour repeats periodically.



Figure 6: Dynamic behaviour of "predator-prey" ecological model (A=Prey biomass, B=Predator biomass)

## 5. Conclusions

In my future work I intend to further improve QSIM predicting method, decreasing QSIM algorithm complexity, by combining qualitative and numerical simulation. It shows that there is a feedback, guiding the numerical simulation towards a satisfactory qualitative behaviour (figure 7), which is at present only manually exploited (potentially automated).



Figure 7: Interaction between numerical and qualitative simulation

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