## Title
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**Authors**
An, Sungeun
Rugaber, Spencer
Weigel, Emily
et al.

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# Cognitive Strategies for Parameter Estimation in Model Exploration

**Sungeun An (sungeun.an@gatech.edu)**
School of Interactive Computing, Georgia Institute of Technology,
Atlanta, GA 30308 USA

**Spencer Rugaber (spencer@cc.gatech.edu)**
School of Computer Science, Georgia Institute of Technology,
Atlanta, GA 30308 USA

**Emily Weigel (emily.weigel@biosci.gatech.edu)**
School of Biological Sciences, Georgia Institute of Technology
Atlanta, GA 30332 USA

**Ashok Goel (goel@cc.gatech.edu)**
School of Interactive Computing, Georgia Institute of Technology
Atlanta, GA 30308 USA

**Abstract**

Virtual laboratories that enable novice scientists to construct, evaluate and revise models of complex systems heavily involve parameter estimation tasks. We seek to understand novice strategies for parameter estimation in model exploration to design better cognitive supports for them. We conducted a study of 50 college students for a parameter estimation task in exploring an ecological model. We identified three types of behavioral patterns and their underlying cognitive strategies. Specifically, the students used systematic search, problem decomposition and reduction, and global search followed by local search as their cognitive strategies.

**Keywords:** parameter estimation; model exploration; modeling and simulation; cognitive strategy; problem-solving

## Introduction

Parameter estimation is a common problem for humans and thus there exists a large literature on addressing it (Brown & Burton, 1978; Kalp, 1995, Varma & Schwartz, 2011). As a simple example from arithmetic, consider the subtraction problem (671 – 28). In early work, Brown & Burton, (1978) identified several types of errors novices make in calculating the results of such subtraction problems. Kalp (1995) described general cognitive strategies for addressing such problems: problem decomposition that partitions the subtraction problem into subproblems; sorting that prioritizes search in the resulting problem spaces; and problem reduction that solves and eliminates sub-problems. Kalp (1995) also presents a parameterization technique that composes the solutions to the subproblems into a solution for the whole problem under the assumption of piecewise linearity of the functions in the subproblems.

As an example of more challenging parameter estimation problem, most humans have difficulty calculating the value of √5 without the assistance of an electronic device. Yet, most humans can correctly estimate its value as a real number between 2 and 3 that is closer to 2 than to 3. One cognitive strategy is to map the problem into the dual space of a straight line, imagine integer values on the line, recall that √4 equals 2 and √9 equals 3, use 4 and 9 as anchor points, and recognize that 5 is closer to 4 than to 9 (Varma & Schwartz, 2011). In addressing this problem, people make use of the monotonicity of the √ function, with the straight line acting as a model of the function.

While these estimation problems in arithmetic deal only with a small number of parameters (only one in case of the √ problem), where the range of values a parameter can take is discrete and small (one of ten integers for each column in the subtraction problem), they illustrate a few points (Ashcraft, 1992; Dehaene, 2011): (i) novices often find parameter estimation cognitively challenging, (ii) it is important to understand the cognitive strategies novices use for parameter estimation tasks, (iii) the cognitive strategies for parameter estimation can vary from task to task, and (iv) the cognitive strategies often make assumptions about the linearity or monotonicity of the functions.

The advent of modern informatics–data visualization, interactive machine learning, open learning environments, etc.– often engages humans in parameter estimation tasks in modeling complex systems with high dimensional parameter spaces, where the number of parameters can be large (ten or more) and the range of values a parameter may take can be large (hundreds, thousands, or more). "Virtual laboratories" that enable novice scientists to construct, evaluate and revise models of complex systems in biology and ecology heavily involve parameter estimation tasks (Basu, Biswas, & Kinnebrew, 2017; Bridewell, Sánchez, Langley, & Billman, 2006; De Jong & Van Joolingen, 1998; Sins, Savelsbergh, & van Joolingen, 2005). Using a virtual laboratory, a modeler can examine the influence of a large number of parameters on the model of an ecological system and conduct "What If?" experiments by varying the values of the parameter values. The question then becomes: What are the cognitive strategies that novice modelers use to estimate the parameter values in this high-dimensional space? It is important to understand their cognitive strategies for designing effective cognitive scaffolds and pedagogical techniques (Joyner & Goel 2015).

The literature on parameter estimation is very large, including techniques such as genetic algorithms, neural networks, reinforcement learning, and Bayesian parameterization, etc. Here we will note two points. First, while digital libraries such as the Smithsonian Institution's Encyclopedia of Life (EOL; eol.org) contain knowledge about the parameters of more than a million biological species, they contain little information about the probability distributions of the parameter values of any species (Parr et al., 2016). It is also unlikely that most novice modelers have much background knowledge of the probability distributions of the parameter values for even a small number of biological species. Second, as MacLeod & Nersessian (2018) recently pointed out, our understanding of what cognitive strategies humans use in navigating parameter spaces in modeling complex biological systems is limited (MacLeod & Nersessian, 2018). The present work seeks to add to this modest understanding so that we can build interactive learning environments that can provide cognitive support to novice modelers.

We describe an experimental study using a web-based virtual laboratory in which 50 college-level biology students engaged in the parameterization task for modeling an ecological system in a classroom setting. In this study, the task was deliberately limited to estimating the value of only one parameter, though the value could vary from 1 to 1000. An analysis of students' parameter estimation behaviors showed three different behavioral patterns. The three patterns use differing combinations of systematic search, problem decomposition/reduction, and global/local search. We also related the patterns with successful outcomes on the parameterization task.

## Experiment

In Fall 2019, we conducted an *in situ* experiment in a physical classroom of an undergraduate Introduction to Biology class at a large public R1 institution in the southeastern US.

### Participants

A total of 50 students who attended a 50-minute period of the introductory biology class participated in the study (N=50). Given the nature of the course and the students' self-assessments, the students were novice biologists as well as naive modelers, who had limited biology knowledge or experience in modeling. On a 1-5 Likert scale, the average self-perceived familiarity with biology was 2.80 and the average self-perceived familiarity with modeling was 2.22. The study was conducted as part of the course following an approved IRB protocol, and the students did not receive any monetary compensation or additional course credit for their time.

### Materials

A freely and publicly available web-based virtual laboratory called VERA was used for modeling complex systems during the experiment (https://vera.cc.gatech.edu/; An et al., 2020; An et al., 2021). VERA evolves from earlier work on the ACT (Vattam et al., 2011), EMT (Joyner et al., 2011) and MILA (Joyner, Goel & Papin, 2014) learning environments.

VERA enables a user to interactively build conceptual models of ecological phenomena. Conceptual models of ecological phenomena in VERA are expressed in the Component Mechanism Phenomenon (CMP) language

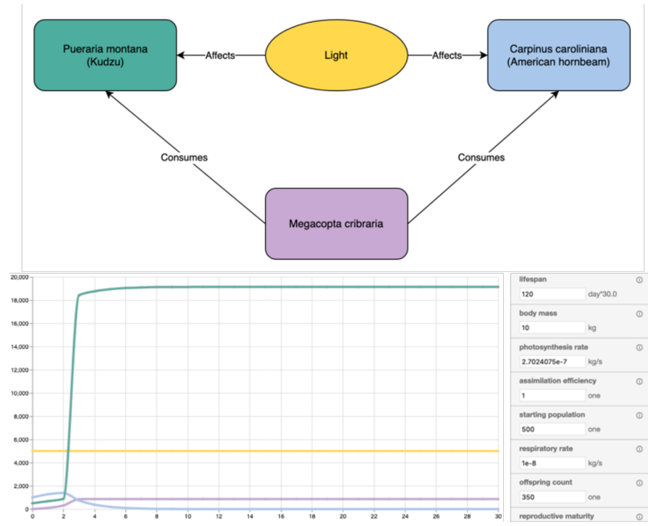


Figure 1: The conceptual model, the simulation parameters of kudzu, and the simulation output generated based on the conceptual model and its parameters. X axis: Time (months). Y axis: Population. The color of lines represents the biotic and abiotic components in the conceptual model.

(Joyner et al., 2011) that derive from the Structure-Behavior-Function theory of modeling complex systems (Goel et al., 2009). A CMP model consists of components and relationships between components. A component can be either biotic or abiotic. A relationship connects one component to another in a directed manner. In Figure 1, the top image shows a conceptual model of the kudzu plant showing interactions among kudzu (biotic), kudzu bug (biotic), American hornbeam (biotic), and sunlight (abiotic).

VERA uses several AI technologies to help users construct, evaluate, and revise their models. First, an AI compiler (Joyner, Goel & Papin, 2014) automatically spawns an agent-based simulation in the NetLogo platform (https://ccl.northwestern.edi/netlogo/; Wilensky & Rand, 2015) directly from the visual syntax and operational semantics of the conceptual model. The bottom image in Figure 1 shows the results of running the NetLogo simulation of the conceptual model shown in the top image. The virtual experimentation through running simulations enables a user to observe the evolution of the system variables over time and iterate through the model generate-evaluate-revise cycles.

Second, VERA provides access to Encyclopedia of Life (EOL; eol.org; Parr et al., 2016) to help construct the conceptual model and set initial values of the simulation parameters. This enables the user to learn domain knowledge in specific contexts and in relation to other domain knowledge.

Third, VERA uses genetic algorithms for parameter optimization to fit the model to the existing data (Broniec et al., 2021). This allows the users to conduct "What If?" experiments with different parameter settings to either explain an ecological phenomenon or attempt to predict the outcome of changes to an ecological system.

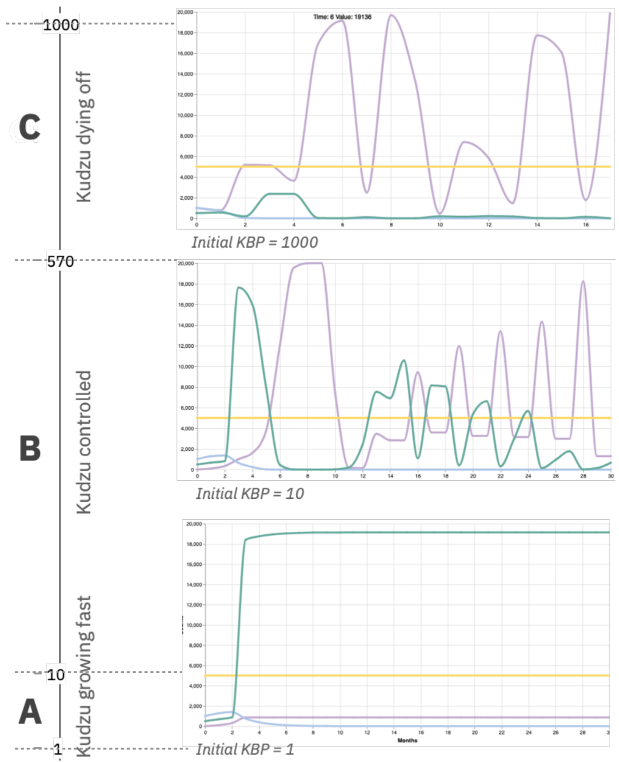


Figure 2: The parameter spaces of kudzu bug population (KBP) and the simulation output graphs for each parameter (Kudzu: green; American hornbeam: blue; Kudzu bug: purple; Sunlight: yellow).

Finally, VERA uses an AI teaching assistant called Jill Watson (Goel & Polepeddi, 2018) to answer a user's questions based on the user guide document. In particular, Jill Watson in VERA provides explanations about both the domain vocabulary knowledge used in VERA (e.g., such as "What is a food web?") and the mechanics of using VERA (e.g., "How do I make a model?") (Goel, 2020).

## Procedure

Before the class intervention day, the students completed a class assignment ('pre-test') to assess their baseline biology knowledge. During the intervention, we spent approximately 15 minutes training the students on the concept of scientific modeling and the use of the system. We walked the students through one case of building, testing and revising a model. Next, the students were instructed to spend 25 uninterrupted minutes to complete a modeling task on a pre-built (kudzu) model (Figure 1). The experiment instructions were embedded in a Qualtrics survey. After the exploration, students completed a class assignment to examine what they learned ('post-test'). The questions on the pre-/post-tests were different but aimed at the same concept. All the students in the class used the VERA virtual laboratory on their own laptops during the study.

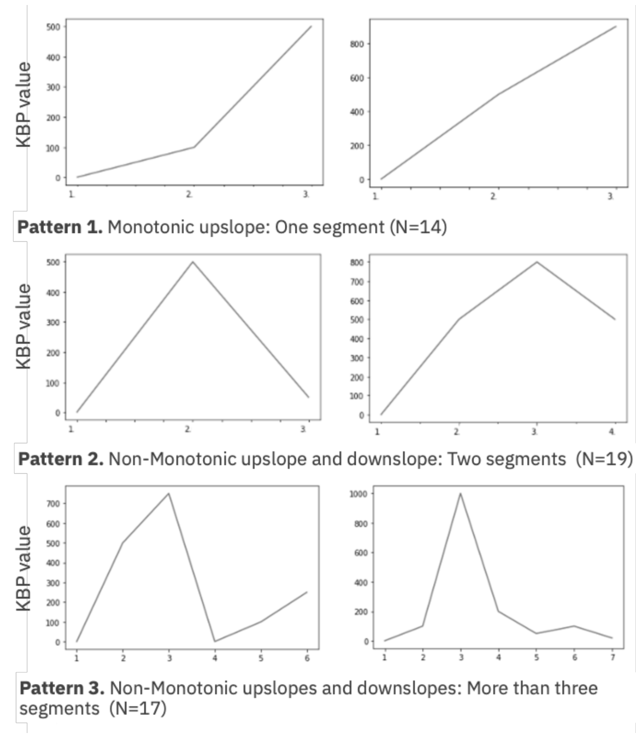


Figure 3: Examples of three different patterns (x-axis: $n^{th}$ attempt; y-axis: the attempted KBP values). For example, the sequence of attempted KBP values in the first graph is 0, 100, 500.

## Parameterization Task

For the modeling task, the students were given the pre-built kudzu model in the VERA system created by the researchers (see Figure 1). The model addresses the invasive species, kudzu (*Pueraria montana*), a fast-growing vine originally from Asia brought to the United States in the late 19th century. Kudzu competes with a native plant, American hornbeam (*Carpinus caroliniana*), for resources like light. Another Asian import, kudzu bug (*Megacopta cribaria*), which feeds on both kudzu and American hornbeam, can potentially slow down the spread of kudzu vines, but also of American hornbeam.

As shown in Figure 2 (but not shown to the students in this study), the size of the kudzu bug population (KBP) on a scale of from 1 to 1000 can lead to three different outcomes. (1) When KBP is between 1-10, kudzu grows fast and outcompetes American hornbeam for the shared resource of light, and American hornbeam does not survive the competition with kudzu (indicated as a blue line). (2) When KBP is between 10- 570, the kudzu population is controlled while American hornbeam also survives. (3) When KBP is between 570-1000, the kudzu and the American hornbeam population both die off due to the large KBP population.

Without knowing the effects of these values, the students were asked to manipulate the KBP to select the best value for the ecosystem stability, making sure that kudzu, the kudzu bug, and American hornbeam all survive, creating a longterm predator-prey cycle. The students were first asked to observe the simulation results of the initial model in which KBP was set to 1 and that manifested a fast-growing kudzu population. Then they were asked to alter the KBP value between 1 and 1000 to estimate what they thought to be the optimal value for the KBP for the ecosystem and to explain their reason in a short text.

The participants' log data was collected through our logging technology while they interacted with VERA. Specifically, we collected their activity logs including the projects and models they created and edited with timestamps. The collected low-level data is then processed to identify the KBP values they have tried for this task.

## Results

We analyzed the 50 students' log data and answers. We identified the three patterns of parameter estimation behaviors shown in Figure 3. We then inferred the cognitive strategies used by the students.

**Behavior Patterns** As shown in Figure 3, three different parameter estimation behavior patterns were monotonic upslope (Pattern 1), non-monotonic upslope and downslope (Pattern 2), multiple upslopes and downslopes (Pattern 3). In the following discussion, a *segment* refers to a section in a pattern that is either upslope or downslope. In Pattern 1, 14 out of 50 students continuously increased the values to estimate the optimal value for KBP. The students in this category started with a relatively small value for KBP and then gradually increased its value and explored its impact on the ecosystem. In Pattern 2, 19 students showed an upslope segment (increasing values of KBP) and a downslope segment (decreasing KBP values). Lastly, in Pattern 3, 17 students explored three or more segments of upslope and downslope segments (corresponding to increasing and decreasing KBP values, respectively).

The students' estimate of the optimal value for KBP determined whether the modeling task was successful or unsuccessful. If a student's answer on the optimal value for KBP was between 10-570, we counted it as successful; otherwise, we assessed it as unsuccessful. Overall, 39 out of the 50 students were successful in finding the optimal value of the kudzu bug whereas 11 students were not. As shown in Table 1, the students who showed Pattern 2 were more likely to be successful in finding the optimal parameter value (89.47%) followed by Pattern 1 (78.57%), and Pattern 3 (64.70%). Within Pattern 3, the students who showed more than four segments were the least successful in estimating the optimal value for KBP; only 3 out of 6 succeeded for a success rate of only 50%.

**Cognitive Strategies** A detailed analysis of the above data suggests that the students in our study showed three distinct cognitive strategies interleaved with one another. The first is systematic search common in problem-solving and found, for example, in searching for information on the web (Tabatabai et al., 2005; White et al., 2007; Aula et al., 2010). Systematic

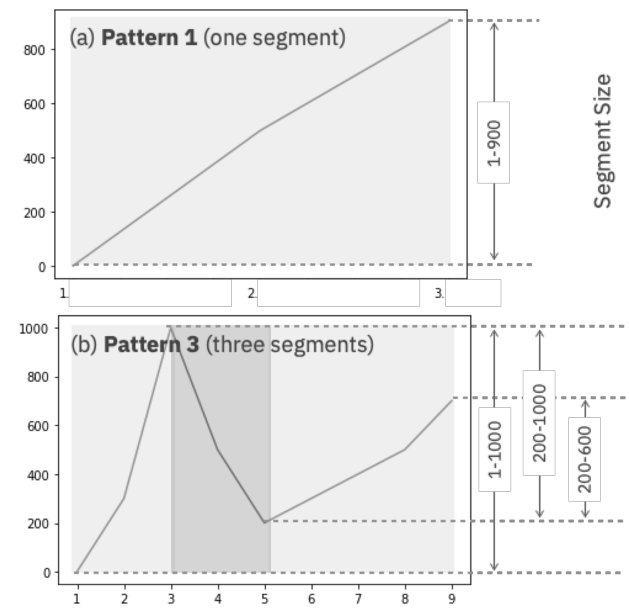


Figure 4: The segment sizes of (a) Pattern 1 with one segment (Top) and (b) Pattern 3 with three segments (Bottom). Light gray region illustrates upslope; Dark gray region illustrates downslope. In Pattern 3, the segment sizes steadily decrease (999, 800, 400).

search takes an initial value and only make monotonic changes with each attempt. For example, it starts with one value for a parameter and then iteratively increases or decreases the value. This is manifested in each linear segment of Patterns 1, 2, and 3, most evidently in Pattern 1.

The second strategy is problem decomposition and reduction (Kalp, 1995; Jacobson, 2000; Hogan & Thomas, 2001). Problem decomposition partitions the overall problem into smaller and simpler subproblems and problem reduction (which address some subproblems thereby reducing the overall problem). Figure 4 illustrates the pattern estimation behavior resulting from this strategy. The top graph in the figure represents an example of Pattern 1 and the bottom graph represents an example of Pattern 3. The upslope segments are illustrated by the blue region whereas the downslope segment is illustrated by the red region. Pattern 1 consists of one upslope segment, and the segment size is expressed as the vertical line next to the graph (e.g., 899). The segment size is defined by the difference between the starting value and the ending value of the segment. Pattern 3 consists of three different segments, and the three vertical lines represent the segment sizes for each segment. For example, the first segment size is 999; the second is 800; and the third is 400, indicating problem decomposition.

The third cognitive strategy is global search followed by local search (e.g., Goldberg et al., 1999). Global search estimates the global optimum for the problem, and then local search helps get closer to the optimum. This strategy is manifested in the decreasing sizes of the problem spaces represented here as 'segment' sizes in the behavioral patterns. As Figure 5 illustrates, the segment sizes tend to decrease gradually for both Pattern 2 and 3, though this is more evident

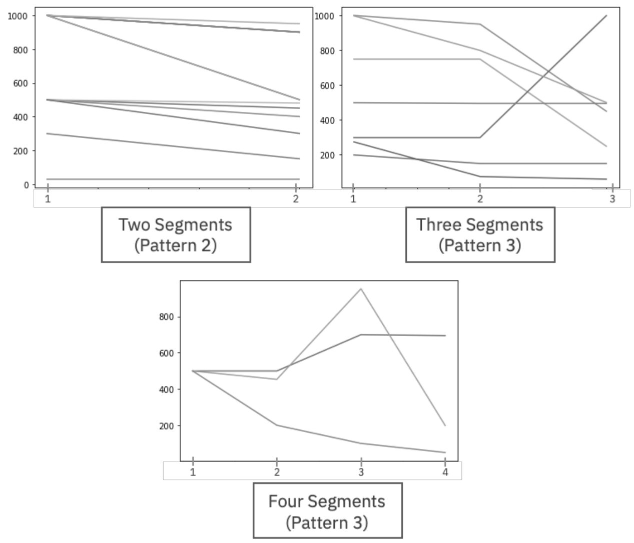


Figure 5: The changes in the segment sizes for the three patterns. X-axis: $n^{th}$ segment, Y-axis: size of the segment. Each line represents a different student. The segment sizes tend to decrease gradually for Pattern 2 (two segments) and 3 (three segments).

in Pattern 2 (two segments) than in Pattern 3 (three or more segments). The above three cognitive strategies were interleaved with one another. This is evident in Pattern 2 that is combining problem decomposition and systematic search.

Statistical analysis was conducted by calculating the slopes of the trend lines for each graph and the trimmed means and the standard deviations were calculated for central tendency. This involves the calculation of the mean after discarding 20% of sample at the high and low ends. As shown in Figure 6, the means of the slopes are negative (Pattern 2 = -150.61, Pattern 2 with three segments = -120, Pattern 3 with four segments = -35.43), which means that the segment size tends to decrease regardless of the patterns.

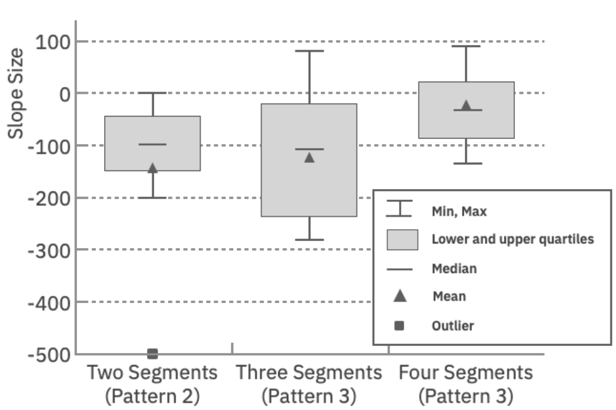


Figure 6: Mean, median, and lower and upper quartiles of the slope sizes of the trend lines for each graph in Figure 5.

**Correlations** Table 1 shows the success rate for three patterns. Briefly, the second pattern resulted in the highest rate of success.

Table 1: The success rate of each pattern.

| | Pattern 1 | Pattern 2 | Pattern 3 |
|---|---|---|---|
| Success rate | 78.57% (11/14) | 89.47% (17/19) | 64.70% (11/17) |

We compared students' academic performance with their parameter estimation behaviors. We found no significant differences among the patterns they used for model parameterization and their self-assessed familiarity with biology as determined by one-way ANOVA ($p$=0.18), or their self-assessed familiarity with modeling ($p$=0.42), or their performance on the biology test ($p$=0.88) (see Table 2). We did find a significant correlation between the cumulative GPA and the parameter estimation behaviors ($p$ <0.05): Pattern 2 has the highest mean value for the cumulative GPA, followed by Pattern 1 and then Pattern 3. On one hand, this follows the success rates of three behavior patterns shown in Table 1: Pattern 2 was most likely to result in success, followed by Pattern 1 and then Pattern 3. On the other, it is difficult to draw strong conclusions about this apparent correlation from a single study of modest size. Additionally, it is important to note that correlations do not imply causality and therefore that no causal claims could be made even with a larger sample as this experiment does not include randomization.

Table 2: The means and standard deviations of each pattern for cumulative GPA, performance on the biology tests, and self-perceived familiarity with biology, and the success rate of each pattern.

| | Pattern 1 | Pattern 2 | Pattern 3 |
|---|---|---|---|
| Cumulative GPA | 3.67 (.36) | 3.72 (.41) | 3.27 (.69) |
| | ANOVA: df = 2.0; f value = 3.88; *$p$ <.05 | | |
| Biology Test Performance | 56.18 (12.33) | 58.45 (10.04) | 57.82 (16.29) |
| | ANOVA: df = 2.0; f value = .12; $p$ = .88 | | |
| Familiarity with Biology | 2.57 (.51) | 2.73 (.80) | 3.05 (.82) |
| | ANOVA: df = 2.0; f value = 1.75; $p$ = .18 | | |
| Familiarity with Modeling | 2.14 (.94) | 2.42 (.96) | 2.05 (.65) |
| | ANOVA: df = 2.0; f value = .86; $p$ = .42 | | |

We also investigated whether gender was correlated with parameter estimation behaviors. As Table 3 indicates, 0% of male students displayed Pattern 1 while 40% of female students did; 60% of male students followed Pattern 2 while 29% of female students did; the proportion for Pattern 3 was approximately the same for male students (40%) and female students (31%). Given the modest size of this study (with number of male students = 15), it is not clear if these differences are real or manifestations of sample bias. We did not try to find correlations with other demographic groupings because of their small proportions in our sample.

Table 3: The gender distribution. N(M)=15. N(F)=35.

| | Pattern 1 | Pattern 2 | Pattern 3 |
|---|---|---|---|
| Gender | M 0% (0.15) | M 60% (9/15) | M 40% (6/15) |
| | F 40% (14/35) | F 29% (10/35) | F 31% (11/35) |

## Discussion

Modeling complex systems is cognitively challenging in part because it involves a high dimensional parameter space. Prior studies have found that students typically struggle with defining and manipulating the variables in a system model and with deciding what values to assign to the variables (VanLehn, 2013). Students also have difficulty understanding the indirect effects of manipulating a variable (Hogan & Thomas, 2001). Consequently, students tend to focus on individual variables separately instead of understanding the direct and indirect interactions among the components of a system as a whole (Hogan & Thomas, 2001; Sins, Savelsbergh, & van Joolingen, 2005).

Further, most novices have a strong focus on adjusting model parameters to fit the empirical data without deeply thinking about the system (Sins, Savelsbergh, & van Joolingen, 2005). Similarly, students often fail to adequately evaluate and revise their models because they spend their effort trying to match their model output to some desired output (VanLehn, 2013). Such model-fitting behavior typically results in the generation of low-quality models. When building a model of a large system, modelers often do not include entire sets of interactions due to their limited working memory for model construction and model- based inferencing. Instead, they start from small models that represent a subset of the problem and then build outwards with those. This cognitive strategy makes modelers build less accurate models, but it makes modeling more tractable (Noble, 2008).

While these prior studies examined novices' difficulties in modeling due to the high dimensionality of the parameter search space, they do not investigate why such difficulties emerge or how novices explore the parameter space. The present study investigates how learners manipulate the parameter values and how they use the simulation outputs to guide adjustments to their estimates of parameter values. In addition, previous studies typically used directed observations and verbal protocols to identify the difficulties of novices while working on a modeling task. In this study, we used students' interaction log data for detailed analysis.

Our analysis indicates that students navigate the parameter space in three different patterns that involve differing numbers of linear segments: one segment (Pattern 1), two segments (Pattern 2), and three or more segments (Pattern 3). Students who explore more than four segments were wandering in the problem space. Our analysis also suggests that novices use three distinct but interleaved cognitive strategies for searching the parameter space: (1) systematic search, (2) problem decomposition followed by problem reduction, and (3) global search followed by local search.

Based on the correlation results we have from this limited study (see Table 2 and 3), the cognitive strategies the students used for the model parameterization task appear to be general constructs. It seems plausible that many students have acquired the strategies of systematic search, problem decomposition/reduction and global/local search from previous experiences and are transferring and applying them to the new context of parameter estimation. This suggests many ways for designing pedagogical techniques, instructional materials, and virtual laboratories. For example, pedagogy can help make these strategies explicit so that more students are successful in using them and fewer students are lost wandering in a large parameter space.

## Conclusion

The use of modern informatics in modeling complex systems poses the cognitive challenge of navigating large parameter spaces. While cognitive science has developed a good understanding of cognitive strategies for estimating a small number of parameters in a small range of values, cognitive science research on parameter estimation in modeling complex systems is still at an early stage. In this paper, we examined the parameter estimation task in the context of ecological modeling in which undergraduate biology students were asked to estimate the value of one parameter for making an ecosystem stable.

We found that the students exhibited three patterns of parameter estimation behavior that appear to be arising due to three cognitive strategies: systematic search, problem decomposition/reduction and global/local search. We also found a correlation between the behavior patterns and the outcomes on the parameter estimation task.

This work is an early step in understanding learners' parameterization search patterns and leaves many exciting questions to be answered with further research. Having students explore a more complex space (many components and many parameters) may give us different insights into parameter search strategies. Also, we expect that results can vary by the complexity of the task, for example, a well-defined task as in our study vs. a more open-ended sense-making task.

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