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ABSTRACT

Title of Thesis: A Framework for Predicting and Controlling System-Level Properties of

Agent-Based Models

Donald P. Miner, PhD in Computer Science, 2010

Thesis directed by: Dr. Marie desJardins, Associate Professor
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An ABM is a computational model that simulates a complex system of many autonomous agents. For example, ABMs have been used to model food chains, the spread of disease, traffic situations and flocking animals. All of the behaviors in an ABM, from agent-level local interactions to system-level behaviors, emerge from local interactions, which are governed by the individual agent programs. The behavior of each individual agent in an agent-based model (ABM) is typically well understood because the agents' program has adjustable control parameters that directly modify its behaviors. However, users of ABMs do not typically have an explicit model of how the values of agent-level control parameters affect the observed system-level behavior of the ABM. Because of this lack of a model, the emergent behavior of an ABM is generally reduced to a repetitive process of guess-and-check: select new agent-level parameter values and then observe and evaluate the result. That is, the controller of the system is forced to use the agent-level parameters, which only indirectly affect the system-level behavior. This process is repetative.

This dissertation presents a domain-independent approach for modeling how changes in agent-level control parameters affect the system as a whole, and for using this model to enable a user to predict and control the behavior of the system *at the system level*. The approach is implemented as a learning-based framework, named the ABM Meta-modeling Framework, for defining correlations between agent-level parameter values and quantitative system-level behavior. Regression methods such as k-nearest neighbor, locally weighted scatterplot smoothing, and nonlinear least squares are used to predict system-level property values, given the system configuration. The mappings from agent-configuration space to system-level behavior space are then inverted with a novel approach to produce inverted predictions that suggest system configurations, given desired system-level property values. The effectiveness and flexibility of the ABM Meta-modeling Framework are demonstrated with experiments from four diverse ABMs implemented in NetLogo, a popular multi-agent programmable modeling environment.

A Framework for Predicting and Controlling

System-Level Properties of Agent-Based Models

by

Donald P. Miner

Thesis submitted to the Faculty of the Graduate School
of the University of Maryland in partial fulfillment
of the requirements for the degree of
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2010

This dissertation is dedicated to my father, my mother, and my wife.

Thank you for your unending love and support.

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Dr. Richard Chang introduced me to my first research experiences and motivated me to tackle hard problems. Since taking algorithms with him in my undergraduate studies and completing my undergraduate thesis with him as my advisor, Dr. Chang has been a great friend and a great person to go to for advice.

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The graduate student community at UMBC is a wonderful support group. I would like to thank graduate students and post-docs Dr. Jesus Caban, Wes Griffin, Yasaman Haghpanah, Dr. Josh Jones, Niels Kasch, James MacGlashan, JC Montminy, Sourav Mukherjee, Patti Ordonez, Soumi Ray and Brandon Wilson for their support.

Dr. Bill Rand and Forrest Stonedahl introduced me to NetLogo and much of the agent-based modeling terminology used in this dissertation. My research was not focused on any particular type of system before meeting them. My work naturally found its home in ABMs and NetLogo, which overall made my research far better than what it would have been otherwise.

I was assisted by undergraduate researchers in various stages of my research. Thanks to Peter Hamilton, Kevin Winner, Doug Still and Nathaniel Wise for their contributions.

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Chapter 1

INTRODUCTION AND MOTIVATION

The behavior of individual agents in an agent-based model (ABM) is typically well understood because the agent's program directly controls its local behaviors. What is typically not understood is how changing these programs' agent-level control parameters affect the observed system-level behaviors of the ABM. The aim of this dissertation is to provide researchers and users of ABMs insight into how these agent-level parameters affect system-level properties. I present a learning framework, the ABM Meta-modeling Framework (AMF), that can be used to predict and control system-level behaviors of agent-based models. Using this framework, users can interact with ABMs in terms of intuitive system-level concepts, instead of with agent-level controls that only indirectly affect system-level behaviors.

1.1 Agent-Based Models

Agent-based models are used by scientists to analyze system-level behaviors of complex systems by simulating the system from the bottom up. At the core of these simulations are individual agents that interact locally with other agents and with the environment. All of the behaviors in an ABM, from agent-level local interactions to system-level behaviors, emerge from these local interactions, which are governed by the individual *agent programs*.

ABMs can be used to understand how changes in individuals' *agent-level parameters* affect *system-level properties*.
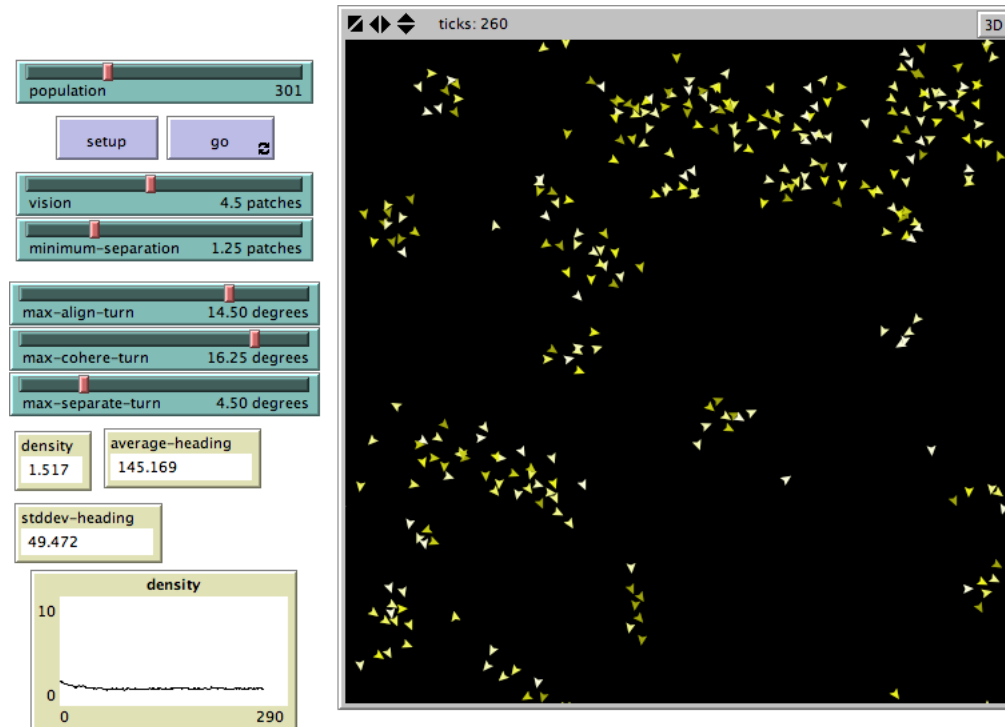
FIG. 1.1. A screenshot of NetLogo's graphical user interface while executing a flocking simulation.

Agent-level control parameters adjust the behaviors of agent-based programs. However, scientists are not typically interested in the local interactions between agents—they are interested in the resulting system-level behaviors that result. For example, researchers studying agent-based models of lane formations in army ants were interested in the traffic patterns of the lanes, not in the individual behaviors of the ants (Couzin & Franks 2003). In other work, researchers studying locusts were interested in identifying the critical density at which locusts would begin to swarm and destroy crops (Buhl *et al.* 2006). Typically, scientists analyze ABMs by viewing visualizations of the environment or by gathering statistical data on the simulation. For instance, NetLogo, an agent-based modeling programming en-

vironment (Tisue & Wilensky 2004), provides monitors, plots, and visualizations to convey system-level properties to the user. In Figure 1.1, monitors are displaying *density*, *average-heading* and *stddev-heading* statistics for a flocking domain. In addition, a plot of density shows how this property has changed over time. These tools can be used by researchers to generate a mental model of how the agent-level control parameters of the flocking domain (the sliders seen in the user interface) affect these system-level properties.

Although using ABMs for researching agent-based systems has been proven useful in a number of domains, there is a major conceptual disconnect, from the user's perspective, between the agent-level controls and the system-level properties. The classical ABM control method of adjusting agent-level properties is unintuitive, because these properties only indirectly affect the system-level properties through emergence. With the current methodology, a simulation has to be executed in order to observe what the values of the system-level properties will be. A time-consuming iterative process of guess-and-check is the only way to configure the system to have it exhibit a desired system-level behavior. Determining what an ABM will do at a system-level, given only the agent-level parameters, is not possible with current software.

The main goal of the ABM Meta-modeling Framework is to bridge the gap between agent-level parameters and system-level properties. AMF reduces the learning curve of an agent-based model, since users are interacting with the system at the system level, instead of at the agent level. Qualitative analysis of an ABM's system-level properties will be a more efficient process using AMF, since researchers can interact with an abstraction of the system's controls. In addition, the models learned by AMF can be inspected to gather quantitative data about the correlations between system-level properties and agent-level parameters.

1.2 Wolves, Sheep and Grass

FIG. 1.2. A screen shot from NetLogo's Wolf Sheep Predation model.

Throughout this dissertation, I will use NetLogo's Wolf Sheep Predation model (Wilensky 1997e), which is bundled with NetLogo's standard Model Library,[1] as an example to explain concepts. A snapshot of its NetLogo visualization is shown in Figure 1.2. This multi-agent model simulates a food chain consisting of wolf agents, sheep agents and grass in a two-dimensional space. The model is controlled by seven agent-level control parameters, which directly affect the following agent behaviors:

- The system is initialized with *initial-number-sheep* sheep and *initial-number-wolves* wolves.

- Wolves and sheep move randomly though the space.

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[1]http://ccl.northwestern.edu/netlogo/models/WolfSheepPredation

- Wolves and sheep die if they run out of energy.

- Wolves eat sheep if they occupy the same space in the environment. Wolves gain *wolf-gain-from-food* units of energy from eating sheep. The sheep dies.

- Sheep eat grass if they are on a location of the environment that has grass. Sheep gain *sheep-gain-from-food* units of energy from eating grass. The grass dies in that grid location.

- Every time step, each sheep and each wolf has a chance (*sheep-reproduce* and *wolf-reproduce*) to reproduce asexually. Both the parent and the child split the parent's original energy evenly (i.e., the parent's energy divided by two).

- Grass regrows after *grass-regrowth-time* number of time steps.

The system-level concepts we are interested in are the number of sheep, the number of wolves, and the number of grid locations containing grass. In NetLogo, these properties are displayed with monitors and a plot, as seen in Figure 1.3. The number of each population of agents may change continuously, but the *average* number of sheep converges. That is, as more values for the sheep populations are sampled, the average approaches a single value, instead of oscillating like the instantaneous population. Another interesting feature is that some ecosystems fail: sheep and/or wolves go extinct.

After working with this ABM for some time, a user will begin to realize that changes in the control parameters will yield different types of behavior. For example, by setting *sheep-gain-from-food* to 2, 3, and then 4, major differences in system-level behavior are apparent, as seen in the graphs in Figure 1.4. When the value of *sheep-gain-from-food* is 4, the system rhythmically exhibits major changes in all three agent populations. When the value is 2 or 3, the population remains relatively stable, but the average population values are different. When the value is low enough (e.g., 2) the wolves go extinct.
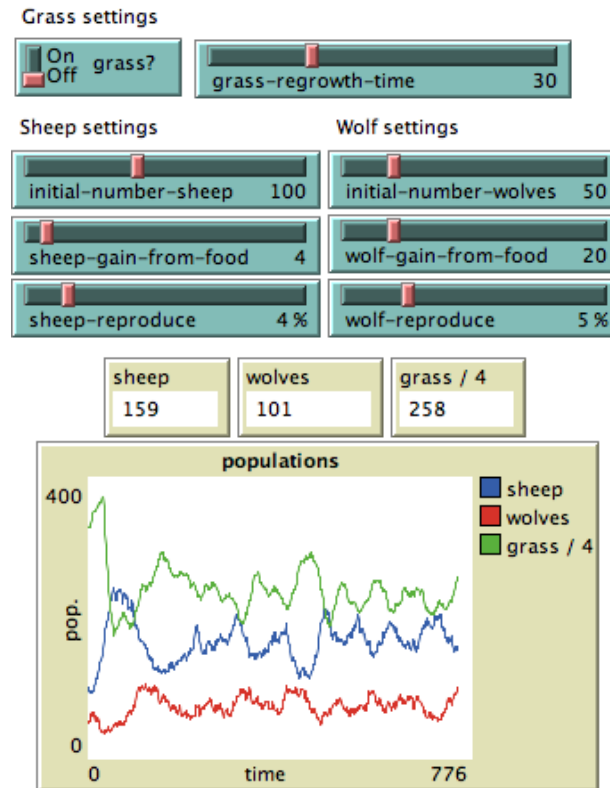
FIG. 1.3. The control and monitor interface for the Wolf Sheep Predation model.

The Wolf Sheep Predation model is a good example of the intuitive disconnect between agent-level parameters and system-level properties. There is no clear *explicit* relationship between the controls presented in the user interface and the resulting system-level properties. An experienced user may have a qualitative understanding of the correlations, but would not be able to predict quantitative concepts, such as the average number of sheep after 2000 time steps (i.e., instantaneous population amounts divided by the number of instantaneous populations sampled). In Chapter 8 (Results), I will show that the intuitive disconnect in this domain can easily be solved by AMF.

sheep-gain-from-food = 4

sheep-gain-from-food = 3

sheep-gain-from-food = 2
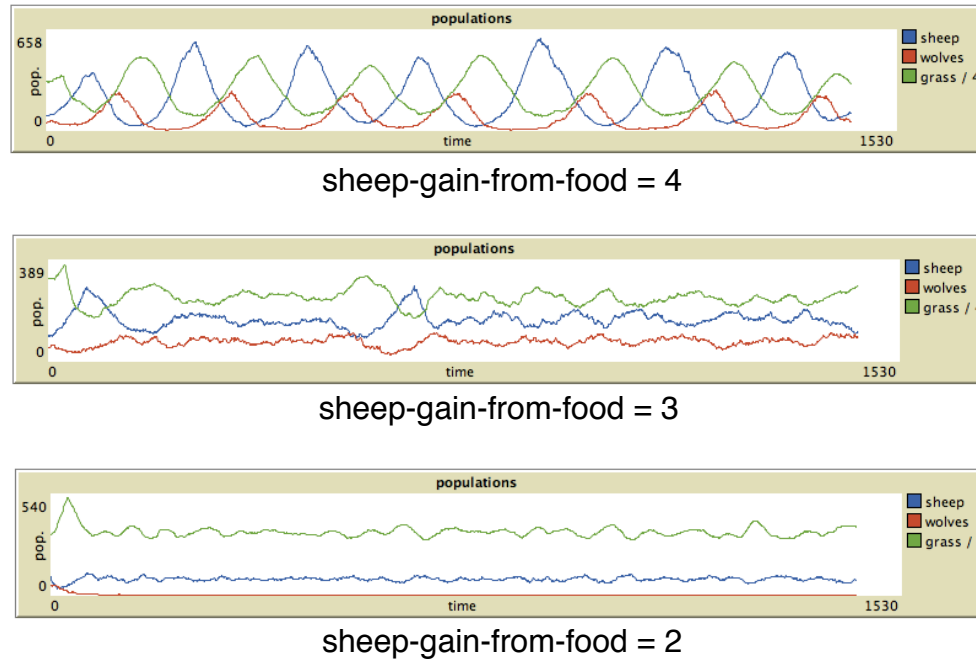
FIG. 1.4. Differences in populations based on changes of the *sheep-gain-from-food* parameter.

1.3   Overview of the ABM Meta-modeling Framework

The foundation of this work is framing the problem of building a meta-model of an ABM as two sub-problems: the *forward-mapping problem* and the *reverse-mapping problem*. In Chapter 6 (The Forward-Mapping Problem), I will discuss how AMF maps given values of the agent-level parameters to expected system-level property values with standard regression approaches. In Chapter 7 (The Reverse-Mapping Problem), I will discuss how AMF maps a set of desired system-level property values to a set of agent-level parameters that would generate this behavior. My general approach to solving the reverse-mapping problem is to interpolate configurations using the forward mapping to approximate a smooth and continuous surface. This interpolated surface represents the space of

configurations that would satisfy the system-level requirements set out by the user. Also, in Chapter 7, I will discuss alternative methods for solving the reverse-mapping problem.

AMF is simple and has only a few configuration points. This allows researchers to focus on the analysis of the system, instead of on the details of AMF. The framework consists of three major steps: sampling, solving the forward-mapping problem, and solving the reverse-mapping problem. In these three steps, the only configurations the user must perform are to define how to measure system-level properties of interest, to provide the ranges of parameters to be sampled, and to select a regression algorithm.

I will show in Chapter 8 that my framework is able to generate models of system-level behavior. For example, AMF is able to predict the average number of sheep and wolves in the Wolf Sheep Predation model, given the configuration parameter values (the forward-mapping problem). Also, AMF is able to make suggestions for the values for the control parameters, given the desired system-level property outcome (the reverse-mapping problem).

A more comprehensive overview of AMF is provided in Chapter 2.

1.4   Summary of Contributions

The main contribution of this dissertation is an in-depth analysis of meta-models of agent-based models. This analysis includes a discussion of methods for using regression to build models of the correlations between agent-level parameters and system-level properties. In addition, this dissertation contains a survey of ways in which meta-models can be used to inspect system-level behaviors of agent-based models.

The ABM Meta-modeling Framework encapsulates my methodology for building meta-models of ABMs. The implementation of AMF serves as a proof-of-concept to show that my approach is feasible and applicable to a variety of domains. The software itself is

a contribution, since it is available to be used by researchers interested in building meta-models of NetLogo ABMs. The design of the general framework is a contribution as well, since it could be implemented to interact with other agent-based modeling systems similar to NetLogo, or totally independent agent-based models.

1.5 Dissertation Organization

This dissertation is divided into nine chapters, including this one. Chapter 2 The ABM Meta-modeling Framework explains each framework component in detail, describes how a new user would tailor AMF to a new ABM, discusses implementation details and gives an introduction to the forward- and reverse-mapping problems. Chapter 3 provides information about NetLogo and algorithms used by AMF. Chapter 4 discusses the numerous different ways that system-level properties of ABM can be defined. Chapter 5 enumerates the domains that AMF has been applied to, along with definitions of system-level properties. Chapters 6 and 7 discuss my solutions to the forward- and reverse-mapping problems. Chapter 8 evaluates AMF on a domain-by-domain basis and provides explicit examples of how AMF has been used. Chapter 9 compares and contrasts related approaches to AMF. Chapter 10 summarizes this dissertation, provides additional discussion and presents possible directions for future work.

Chapter 2

THE ABM META-MODELING FRAMEWORK

The ABM Meta-modeling Framework builds meta-models that map the values of agent-level control parameter values to system-level property values, and vice versa. Learning these mappings are separate problems, which I call the *forward-mapping problem* and the *reverse-mapping problem*. To solve these problems, a user of AMF "plugs in" a regression algorithm of their choice. The framework uses this regression algorithm to learn the mappings and then provide the user with interfaces to query them. Once the mappings are learned, the user can query either for *prediction* or for *control*. A prediction query uses the forward mapping to determine values for the expected values for system-level properties, given the system's configuration. A control query uses the reverse mapping to suggest values for agent-level parameters, given desired values for system-level properties. Most of the implementation details and inner workings of AMF are abstracted away from the user, who only has to attend to a limited number of configuration points.

In this chapter, I will discuss the design goals of AMF, the framework structure, software implementation details, and how well AMF conforms to the design goals.

2.1 Design Goals of The ABM Meta-modeling Framework

My specific goal in designing AMF was to make the process of controlling and interacting with agent-based models more intuitive. In addition to this central goal, AMF strives to be:

- Domain independent: The design of AMF should minimize the amount of configuration that is needed for each new domain;

- Algorithm independent: any regression algorithm should be able to be applied with AMF;

- Accurate: AMF should generate accurate predictions and control suggestions; and

- Fast for the user – interactions with the models generated by AMF should require minimal computational time.

Domain independence is paramount because of the variety of ABMs. I have designed AMF in such a way that the same general approach would work for any ABM. Also, I strove to minimize the amount of configuration that is needed to apply AMF to a new domain. These constraints I have set on the design make AMF broadly applicable to a number of domains, without the need for in-depth domain knowledge. To reinforce this claim, I have tested AMF on a number of diverse domains, using the same general approach for each.

Algorithm independence in a learning framework is important because different algorithms may be more effective for modeling different agent-based models.[1] In addition, algorithm independence allows AMF to scale with new advances in machine learning research, since future state-of-the-art regression algorithms can be used just as easily as current approaches.

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[1] In general, the learning algorithms that will be discussed in this dissertation will satisfy the requirements for modeling most ABMs. However, an in-depth analysis of which types of algorithms should be used for different classes of ABMs is outside the scope of this dissertation research.

Accuracy and fast user response time appear to be obvious design goals. However, achieving these goals require sacrifices in performance in other portions of the framework. AMF requires a significant amount of computational time to sample different configurations of the target ABM. These large training sets can be used to build static meta-models of ABMs that are both accurate and fast to query. In contrast, an active learning approach would be able to learn models faster, but would require more interaction with the user, increasing the user's effort. Likewise, optimization approaches (e.g., hill climbing) could be used to generate arbitrarily accurate results, but typically require numerous iterations and would significantly increase the response time for a user's query, because each step would have to run the ABM to calculate each fitness score, which could take several seconds. In summary, I am making the assumption that users studying ABMs with AMF are more interested in achieving more accurate results for their research and interacting with the models quickly, than spending less time sampling.

2.2 Framework Structure

The framework is split into several phases: sampling, solving the forward-mapping problem, solving the reverse-mapping problem, querying for prediction, and querying for control (i.e., suggesting a configuration). Figure 2.1 shows how the different phases interact with one another. Sampling makes observations from the actual ABM and then feeds the newly generated data set to the forward-mapping solver. The result of solving the forward mapping is a function f, which is used to predict behavior and to develop the reverse mapping f^{-1}. From an external perspective, the framework only has a limited amout of input and output: AMF takes in observations of an agent-based model and provides interfaces to query for prediction and control. The user queries AMF to interact with the agent-based model in an intuitive way.

Many configuration points exist, which allow users of AMF to modify the behavior of the framework. However, the individual phases take the same output and provide the same output, regardless of the configuration. This uniformity is what makes AMF a framework and not simply a collection of algorithms. For example, even though different regression algorithms can be used to learn the forward mapping, the forward mapping always provides predictions of how an ABM will behave, from the user's perspective.

2.2.1   Defining System-Level Behavior Properties

The system-level properties of an ABM must be defined by the user of AMF. The measurement of a system-level property is a statistical or mathematical calculation based on the state of the ABM over some period of time (or "ticks"). The one assumption made by AMF is that the measurement is *stable*, meaning that as the same configuration is sampled repeatedly, the measurement's value should vary minimally. One way to measure stability is to calculate the standard deviation of measured values of several runs of the same system. The need for this assumption, ways to conform to it, and a more detailed explanation of how to define system-level properties is provided in Chapter 4.

For example, there are several system-level behavior properties that can be measured in the Wolf Sheep Predation model. Three of the most obvious properties are the average number of sheep, average number of wolves, and average amount of grass over a significant number of ticks. These are measured by individually summing the number of sheep, wolves, and grass living at each time step and dividing by the number of ticks. Although the number of sheep and wolves change rhythmically, the average values typically converge to a single value after about 10,000 ticks.
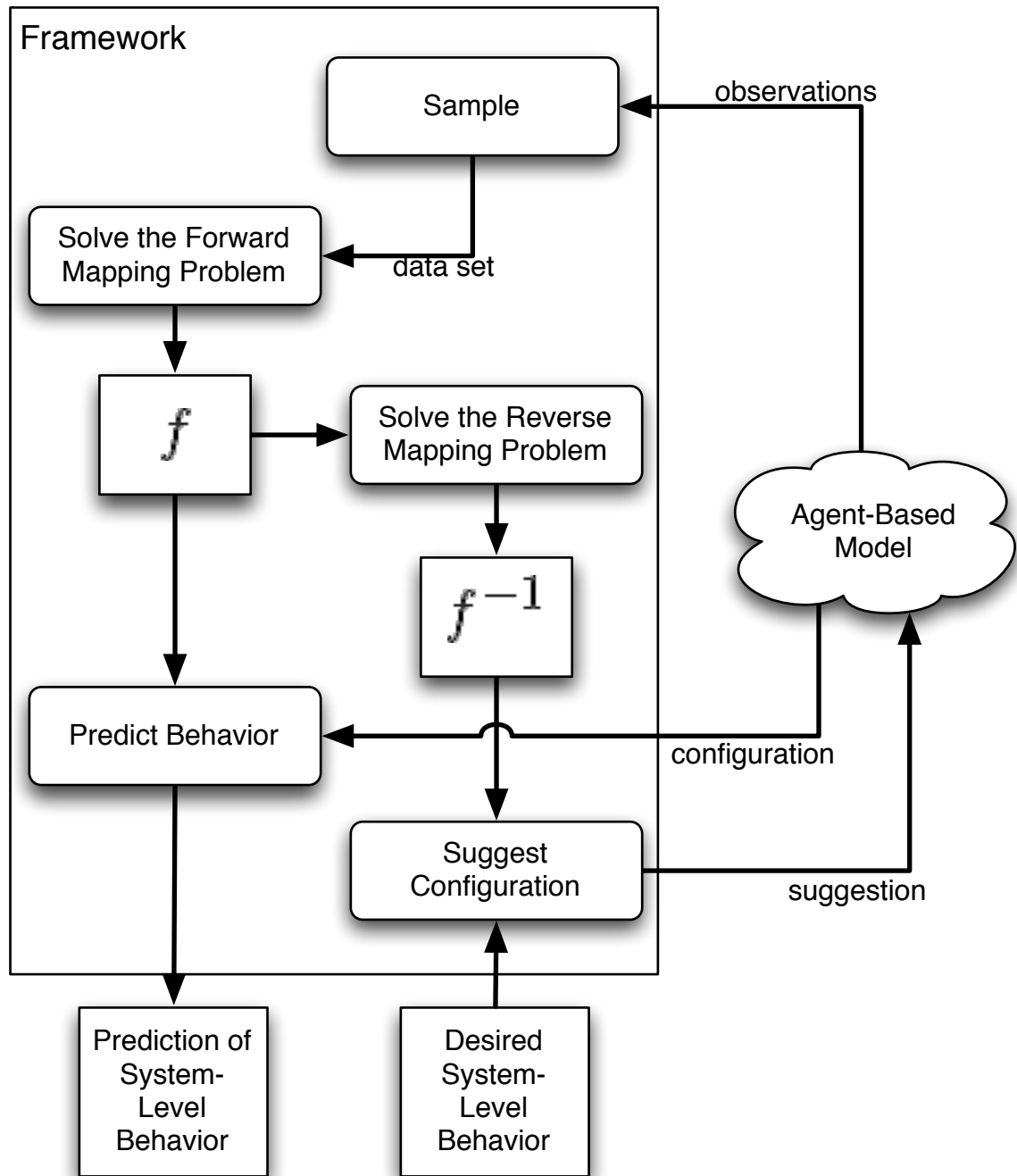
FIG. 2.1. An overview of the phases of AMF and how data flows among them.

2.2.2   Sampling

The first phase is *sampling*. In this phase, numerous observations are made of different configurations of an agent-based model. A data set is generated that contains the independent variables (the agent-level control parameter values) and the resulting system-level behaviors, for each observation. This process can be very time-consuming, depending on several factors:

- Execution time of the model – the models will be executed numerous times, so the longer a model takes to execute, the longer the whole set of experiments will take to execute.

- Granularity – more fine-grained sampling will take more time, since more points must be sampled.

- Dimensionality – more agent-level control parameters result in a larger search space and naturally more points to sample.

A 120-observation sample of the NetLogo *Fires* model[2] (Wilensky 1997d) requires about thirty seconds[3] to generate. A large sample of 50,000 observation of a Reynolds boid flock (Reynolds 1987) took approximately four days.

The user is required enough understanding of the domain to specify to AMF which ranges of values should be sampled. AMF is not able to automatically infer which value ranges are interesting, so these must be explicitly defined.

This sampling process is easily parallelizable. Since each experiment is independent of the others, the set of all experiments can be segmented among a number of systems and processors to significantly reduce the computation time. Once all of the experiments are completed, the results can be merged into one data set.

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[2]See Chapter 8 for detailed results.
[3]Most experiments are executed on a 3.0 Ghz Pentium 4 running Arch Linux.

For the purposes of this dissertation, I limit AMF to use a simple random sampling method (i.e., randomly select points within a specified range) or a systematic sampling method (i.e., given ranges, sample evenly spaced points). I acknowledge that intelligent sampling strategies could improve the performance of the framework, and such strategies could be the focus future work.

2.2.3 The Forward-Mapping Problem

The *forward-mapping problem* is to develop a function $f : \mathbb{R}^n \to \mathbb{R}$ that maps a provided configuration vector $\mathbf{x} = \{x_1, x_2, ..., x_n\}$ to several system-level behavior properties $\hat{\mathbf{y}}$:

$$f(\mathbf{x}) \to \hat{\mathbf{y}}$$

The set of values $\mathbf{x}$ consists of all the agent-level parameters (independent variables) in the data set provided by the sampling phase. An individual mapping is learned for each system-level behavior measurement provided by the user.

This problem is solved with straightforward regression, such as k-nearest neighbor. In this phase of AMF, the regression algorithm is first "initialized," if necessary. For example, linear regression would need to solve the least-squares problem. Meanwhile, an algorithm like k-nearest neighbor would not necessarily need to initialize anything because it scans the data set per query. Then, the forward mapping can be used to predict values for configurations that have not been sampled.

Once this phase is completed, the user is presented with f, an interface to the mapping built by the regression algorithm. The forward mapping is primarily used to *predict* what the system-level property values will be, given the system's configuration. For example, a learned mapping could be used to determine the average number of sheep given a configuration vector, without having to run the system. Some sample predictions, given particular

system configurations, are shown in Table 2.1. The values for a system configuration represent *grass-regrowth-time*, *sheep-gain-from-food*, *wolf-gain-from-food*, *sheep-reproduce*, and *wolf-reproduce*, respectively.

Table 2.1. Sample Predictions of Behavior in the Wolf Sheep Predation Model

Configuration	Average # Sheep	Average # Wolves	Average # Grass
$(30, 4, 20, 4, 5)$	162.8	76.1	964.8
$(30, 3, 26, 7, 5)$	122.8	90.4	1135.2
$(14, 3, 26, 7, 5)$	144.3	163.8	1621.4
$(5, 3, 17, 7, 5)$	946.9	3.4	1065.4

A more in depth definition of the forward-mapping problem, specific examples of regression methods used in AMF, and the role of regression is given in Chapter 6.

2.2.4 The Reverse-Mapping Problem

The *reverse-mapping problem* is to produce a mapping $f^{-1} : \mathbb{R} \rightarrow \hat{S}$ from a given system-level behavior properties $\mathbf{y}$ to a set of configurations $\hat{S} = \{\hat{\mathbf{x}} | f(\hat{\mathbf{x}}) = \mathbf{y}\}$ (i.e., S is the set of behaviors that will produce behavior $\mathbf{y}$):

$$f^{-1}(\mathbf{y}) \rightarrow \hat{S}$$

The problem of developing the mapping f^{-1} is what I call an "inverted regression problem" and has many unique challenges. The main challenge is that f^{-1} does not, in general, describe a functional mapping: f^{-1} describes a one-to-many relationship, since f is many-to-one. Therefore, AMF cannot use standard regression techniques to solve this problem. Instead, the default behavior of AMF is to approximate the inverse of the forward mapping, using a novel method that I developed called *simplical complex inversion*. This approach has the benefit of using the forward mapping to develop the reverse mapping, so

no additional inputs from the user or additional data samples are needed.

The reverse mapping can be used to suggest a system configuration that will exhibit a specific set of system-level properties. I call this process *control* of the ABM, since it is controlling the ABM at the system-level by suggesting configurations. For example, the reverse mapping could be used to suggest a configuration of $(30, 4, 20, 4, 5)$ for a desired system-level property of 162.8 average sheep (see Table 2.1). However, using the reverse mapping is more involved than using the forward mapping, because f^{-1} returns a set of possible solutions, not a single suggestion. If the mapping is to be used for control, any configuration in this set will satisfy the system-level requirements. Therefore, an additional step must be taken to extract a point from the set if it is to be used to control an ABM.

The implementation details of developing reverse mappings and how to use the reverse mappings are discussed in Chapter 7.

2.2.5   Summary of Configuration Points

The following is a summary of the configuration points discussed in this section. For each new domain, the user must specify the following:

- A list of agent-level control parameters, and the ranges within which they should be sampled.

- A list of system-level behavior properties and a process for measuring them.

In addition, the user may configure the following if they wish to modify the default behavior of AMF:

- The sampling strategy (default: random sampling).

- The regression algorithm to be used for the forward mapping (defaults: k-nearest neighbor, locally weighted linear regression, or nonlinear regression).

- The method for the reverse mapping (default: approximate the inverse of the forward mapping).

2.3 Software Implementation Details

So far, I have discussed AMF abstractly, avoiding specific implementation details because the framework is a methodology and could be reimplemented in a number of different ways or to work with a number of different ABM simulation systems. In this section, I discuss the details of my proof-of-concept implementation that was used to run many of the experiments documented in Chapter 8.

I have tested AMF with NetLogo[4] domains, however, technically any agent-based modeling system would suffice. The rest of the framework is implemented in Python. Each step of AMF returns its result as a file, so that it can be passed to the next step or saved for later use. For example, the forward mapping writes the model to a file so that it can be used by both the prediction script and the reverse mapping script.

Since each domain has different variable names and nuances, the user must implement a Java program that interacts with NetLogo's API. An abstract base class for interaction is provided to guide the development of this program. Next, the user lists the configuration parameters and the ranges of these values so that the sampling can begin. Measuring the system-level parameters can either be calculated within NetLogo or in Java. For example, I modified the standard Wolf Sheep Predation model to keep track of the number of sheep at each tick. Then, to extract the value, NetLogo's API is used to retrieve the sum of the sheep divided by the number of ticks. A similar calculation could be performed within a Java program by retrieving each of these values individually, then performing statistics on them. Performing the statistics calculations in Java has the benefit of not having to change

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[4]More about NetLogo is discussed in more detail in Chapter 3.

the NetLogo ABM source code.

During sampling, the data set is written to a file, row by row. Therefore, the results of several instances of the sampling, executing on different machines, can be easily concatenated.

The regression algorithms used with AMF must conform to a standard API and are passed as arguments into the forward mapping, reverse mapping and prediction scripts. Therefore, no configuration of these core scripts is needed, since they are "pluggable."

An overarching "master script," written in Python, runs all steps automatically, limiting the amount of direct interaction with the framework software.

In addition to the core framework software, I have developed a toolkit that queries the models generated by the forward- and reverse-mapping models. The core tools include:

- Query the forward mapping for a prediction by passing in a configuration,

- Query the reverse mapping for a set of possible solutions by passing in a desired system-level behavior configuration,

- Visualize the mappings.

2.4   Analysis of AMF vs. the Design Goals

In this section, I align the actual implementation of AMF with the design goals.

Domain independence— My framework's implementation is domain independent, to an extent. AMF reduces the forward-mapping problem to a classical regression problem of learning the correlation between the agent-level parameters and the system-level properties. My reverse-mapping problem solution is also domain independent because it interacts exclusively with the forward mapping, which is domain independent.. However, my implementation of AMF still requires the user to specify the agent-level parameters and how to

measure the system-level properties. This is a reasonable requirement, since automatically detecting configuration points and having a computer determine the behaviors of interest in an ABM would be a challenging unsupervised learning problem.

Algorithm independence— Any regression algorithm can be plugged into my implementation, as long as it conforms to the standard API. A simple Python wrapper can be written to adapt an existing third-party regression algorithm to work with my implementation of AMF. My default process of inverted regression requires nothing special of the regression algorithm, because the inversion learning process uses the algorithm's standard forward-mapping behavior.

Accuracy— No extra error is incurred by AMF itself; the accuracy of AMF depends on the regression algorithm used and the amount of time spent sampling. If AMF is not providing accurate results with state-of-the-art regression algorithms, either the correlations cannot be learned with current technology or not enough time has been spent sampling.

Fast for the user— Most computation time is spent sampling and learning the models. These operations are offline and do not affect the response time of real-time interaction with the user. The response time of the forward mapping and the reverse mapping are depend on the running time of the regression algorithms, but typically require less than a few seconds.

Chapter 3

BACKGROUND

The purpose of this chapter is to provide necessary background information for understanding concepts related to the ABM Meta-modeling Framework. In contrast to Chapter 9, the previous research presented in this chapter do not share the same motivation as AMF, but provide a foundation upon which AMF builds.

AMF uses preexisting research in two major areas: agent-based modeling and regression. Section 3.1 discusses what an ABM is, discusses some examples of ABMs, and lists some existing multi-agent software frameworks. Section 3.2 defines regression, outlines favorable and unfavorable properties, and describes a number of regression algorithms that have been incorporated into AMF.

3.1   Agent-Based Modeling

Agent-based models are computer simulations that are implemented from an agent perspective. Agents in ABMs are typically(Epstein 1999):

- bounded by a limited global view;

- only able to perform local interactions, affecting their local environment and neighboring agents;

- autonomous (i.e., there is no top-down control); and

- heterogeneous (i.e., agents within the system can have different properties) .

This paradigm stand sin contrast to implementing the system from the "observer" perspective, in which an overarching control system dictates what agents are to do. For example, in NetLogo, an agent moves forward two units with the following command:

```
> fd 2
```

Notice that this code is agnostic to the global direction of the agent or the position of the agent in the environment. The code simply tells the agent to move forward two units. In contrast, if this were to done from the observer perspective in NetLogo, the following code would be necessary:

```
> set [xcor] of turtle 0
([xcor] of turtle 0 + 2 * cos([heading] of turtle 0))
> set [ycor] of turtle 0
([ycor] of turtle 0 + 2 * sin([heading] of turtle 0))
```

This code computes the change in the x-coordinate and the y-coordinate, given that the agent should move 2 units. Then, it adds the result to the agent's original x- and y-coordinates. Finally, it sets this turtle's x- and y-coordinates to the new x- and y-coordinates. This process is cumbersome. The agent-based property of models provides an intuitive way to build multi-agent systems.

One of the common uses of ABMs is to discover which local interactions generate a given emergent behavior of a system through experimentation. The research question is posed well by Epstein as the *Generativist's Question*:

How could the decentralized local interactions of heterogeneous autonomous agents generate the given regularity?

To answer this question, Epstein then poses the *Generativist's Experiment*:

> Situate an initial population of autonomous heterogeneous agents in a relevant spatial environment; allow them to interact according to simple local rules, and thereby generate—or "grow"—the macroscopic regularity from the bottom up. (Epstein 1999)

If a model accurately generates the emergent behavior of the target system, then that ABM could provide a theory for why that behavior emerges. Agent-based models are particularly well-suited to answer the Generativist's question.

Implementing systems as an ABM can be more natural than other approaches when the system cannot be defined in an aggregate manner or when individual behavior is complex (Bonabeau 2002). ABMs are often compared to equation-based modeling (EBM), in which the model is a parameterized system of equations that describe system-level behavior (i.e., the observer perspective). For example, a supply chain management system could be modeled as an ABM or an EBM (Parunak, Savit, & Riolo 1998). In the ABM proposed by Parunak et al., individual agents represent different companies that trade with one another. In contrast, the EBM is a series of ordinary differential equations describing the input and output of different components of the supply network. The authors argue that in this situation, an ABM is more appropriate.

Modeling certain types of behavior, such as changes in state, erratic behavior and local interactions, can prove to be difficult with EBMs. In the NetLogo example above where the agent moves forward, a relatively simple task of adjusting the position of an agent proved to be overly complicated. When more detailed operations need to be performed, the complexity of the observer-perspective model increases dramatically. Agent-based models remedy this difficulty by simply changing the context of the programming.

The concept of ABMs can be extended to other uses beyond modeling. Many swarm intelligence techniques, such as particle swarm optimization (Kennedy & Eberhart 1995) and ant colony optimization (Dorigo 2004), use a decentralized agent-based approach to solve optimization problems. Although they are inspired by naturally occurring phenomena, their purpose is entirely separate from trying to realistically model a multi-agent system.

3.1.1 Examples of Agent-Based Models

ABMs have been used to model a variety of different systems. In this subsection, I outline a number of agent-based models that have been developed by other researchers. These examples will illustrate the uses for ABMs and how they can be used to answer research questions.
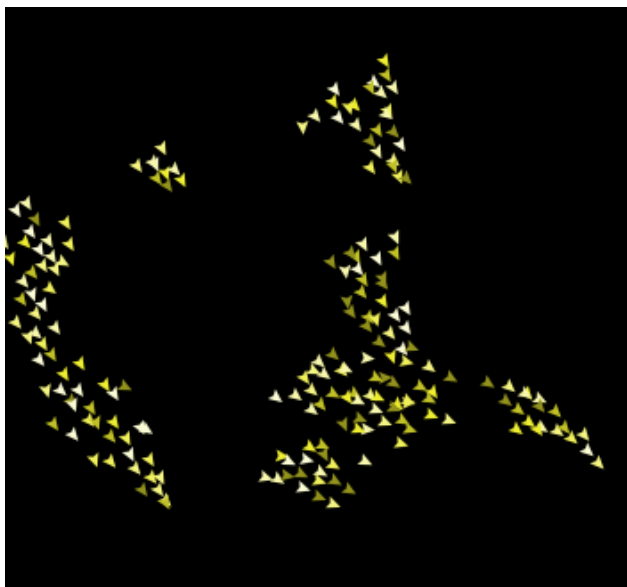
FIG. 3.1. A boid flock moving through a two-dimensional space.

Reynolds Boid Flocking   One of the first popular ABMs was the boid flock (Reynolds 1987; 1999), in which agents move through an environment in a similar way to how birds flock. A screen shot from NetLogo's boid implementation (Wilensky 1997c) is shown in Figure 3.1. Agents follow three simple rules:

- Move away from other agents to avoid collisions,

- Align to move in the same direction as nearby agents, and

- Move towards the central position of local flockmates.

These simple agent-level behaviors result in the elegant flocking behavior observed in a top-down view of the system. This system naturally lends itself to being implemented as an agent-based model because the agents act autonomously and have local interactions with only their neighbors. The flocking behavior is emergent and would therefore be difficult to program directly (e.g., with equation-based modeling).

Boid flocking has been used in a number of applications, such as visualizing time-varying data (Moere 2004), clustering documents (Cui, Gao, & Potok 2006), controlling unmanned air vehicles (Crowther & Riviere 2003), and art (Boyd, Hushlak, & Jacob 2004).

Boids has remained one of my core inspirations for developing AMF. The system is simple, yet exhibits a number of seemingly unpredictable system-level behaviors.

Social Insect Behavior   A number of different computational biology projects have aimed at modeling insect societies. In modeling these systems, researchers are able to gain insights into how individual agent behaviors affect the system-wide emergent behavior. These models are typically based on observations of the real insects.

An agent-based model approach has been used to model how army ants form traffic lanes (Couzin & Franks 2003). The particular species of army ants discussed in this work forms two-way highways to reduce the number of head-on collisions while ants are

searching for food and returning with food. The authors show how the turning rates and perception of the individual ants affect the efficiency of the ants. They found that when the turning rate is too high, ants are too willing to steer off course and intersect the path of other ants. On the other hand, when the turning rate is too low, ants will not adjust their heading to avoid head on collisions. By tuning their model to optimize highway performance, they reached an accurate model of the traffic flow in army ants. The result of this research is an accurate model that describes the individual and group behavior of ants in a traffic situation.

With a different species of ants, researchers were able to produce an agent-based model that simulates the process of an ant colony that collectively selects a location for a new nest (Pratt *et al.* 2005). This process is interesting because an entire ant colony converges on one location, even though many of the ants have only scouted one nest site. Agents are implemented as state machines, in which agents are either exploring for a site, assessing a site, canvassing a site, or committed to a site. In each of these phases, the agent performs different actions and at any time may reject the current site and begin exploring again. Over time, all ants converge on a single site as a nest. With this model, the authors showed that a colony-level decision can be made by ants following agent-based rules.

An ABM has been developed to simulate swarming locusts (Buhl *et al.* 2006). Locusts have an interesting property in that when they are isolated, they tend to not stray from their current location. However, when locusts are among several other locusts, they begin to "march," travelling from one area to another, consuming everything in their path. The authors were particularly interested in determining at what density the locusts begin to march. By changing the number of simulated locusts in a confined space, they were able to determine the critical density at which they would march. This simulation approach is far more practical than experimenting with real locusts. The authors suggest that their models could be used to predict when locust swarms will occur to help warn farmers to protect

their crops.

These particular studies in insect behavior illustrate the need for a system like AMF. Researchers in this field are trying to build theories of how an agent's programming can affect system-level properties. The authors perform empirical studies to answer their research questions and test their hypotheses. However, this approach lacks a robust mathematical understanding of the behavior correlations. Researchers would be able to answer their questions through analytical means provided by a domain-independent approach like AMF to reduce the amount of time spent tailoring specific experiments. More on the comparison this particular type of ABM experimentation and the approach taken by AMF is provided in Section 9.1.

3.1.2 Models of Human Societies

Although human behavior is more complicated than insect behavior, local human interactions can often be generalized to build accurate models of a subset of human society. Most such projects aim to create an accurate model of human interactions with each other in order to predict some society-level behavior.

Agent-based models have been used to determine how locals would react to an incident at the Pacific Missile Range Facility (PMRF) in Hawaii (Zanbaka, HandUber, & Saunders-Newton 2009). The researchers used census data to represent each islander as an individual agent that has either a positive sentiment or a negative sentiment towards the missile facility. Each agents can change its sentiment towards PMRF either by interacting with another agent that has a different sentiment or by experiencing a local event. The model simulates local events and agent interactions and displays how either positive or negative sentiment propagates accross the island. With this model, the authors were able to model hypothetical situations and how they affect the sentiment on the island.

EpiSims is an agent-based simulation tool that models disease outbreaks (Eubank *et*

al. 2004). It uses estimates of how diseases are transmitted and how humans interact based on census and land-use data to realistically simulate human society. The system simulates individuals going to work and shopping, which exposes them to the disease and exposes the disease to others. With this system, researchers are able to predict the effectiveness of mass and targeted vaccination strategies, given a particular community.

STREETS is an agent-based model of pedestrian traffic (Schelhorn *et al.* 1999). Pedestrian traffic is affected by two major aspects: the layout of the street network and the location of attractions. Instead of trying to analyze the behavior of the system from this data alone, STREETS simulates people to determine a number of properties of pedestrian traffic patterns. STREETS initializes the system with a statistically accurate distribution of individuals across the environment. Next, the agent-based model simulates the movement of agents from their arrival point to and through the urban center. Agents visit buildings and attractions and walk among them. Researchers use this tool to observe a top-level view that can be used to analyze the effectiveness of the urban center layout. Hypothetical modifications to the environment can be performed in simulation to determine whether they would improve the traffic situation.

In these simulations, one of the main goals is to model human society so that hypothetical changes can be made to see the changes in the behavior of the system. This way, the researchers do not have to use real humans in social experiments. AMF could be helpful in answering this type of research problem. A desired system-level property could be used to determine suitable configurations by solving the reverse-mapping problem.

3.1.3 Multi-Agent Software Frameworks

Different implementations of different multi-agent systems have many similarities. To reduce the amount of "boiler plate" code for each new multi-agent system, a number of unique multi-agent software frameworks have been developed in the past two decades. In

this section, I survey the most popular of these framewworks. AMF could be configured to analyze ABMs implemented in any of these frameworks.

The Swarm Simulation System   Swarm is one of the original agent-based modeling platforms, originally developed at the Santa Fe Institute in the 1990s. Swarm is currently supported and hosted[1] by an independent organization called the Swarm Development Group. The developers' motivation were to enable researchers to focus less on implementation and more on actual experimentation (Minar *et al.* 1996). To achieve this goal, they implemented a number of libraries in Objective-C and Java that aid in the creation of "swarm" objects, the building blocks of a Swarm simulation. The swarm objects manage the agents and handle the time schedulers that queue the order of agent actions. Also, agents can be nested as hierarchies in swarm objects to allow for heterogeneous collections of agents. Swarm is a discrete time simulation, which means that time progresses as actions occur.

Unfortunately, programming in Swarm can require a significant amount of programming overhead, since the libraries are not a single integrated application (Klein 2003). More recent software frameworks attempt to remedy this situation by providing a more cohesive library of tools.

Repast   The Recursive Porous Agent Simulation Toolkit (Repast) is a comprehensive agent-based modeling toolkit, focusing on modeling social interactions (Collier 2003). The toolkit is freely available to download.[2] Repast is fully object-oriented and attempts to be as platform-independent as possible, supporting programming in Java, Python, Visual Basic.Net, and more.

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[1]The Swarm website: http://www.swarm.org/
[2]The Repast website: http://repast.sourceforge.net/

Repast's feature set is quite comprehensive and extensible. Repast's features are split into six modules (North, Collier, & Vos 2006):

1. The *engine module* controls the agents, environment and scheduler.

2. The *logging module* records execution results.

3. The *interactive run module* manages user interaction with the model.

4. The *batch run module* allows the user to design a series of simulations to be executed in succession.

5. The *adaptive behaviors module* provides built-in adaptive agent behaviors that use techniques such as genetic algorithms and neural networks.

6. The *domains module* helps define environments, such as social systems, geographic information systems, and computational game theory.

All these modules function together to provide a modular programming environment for a diverse set of multi-agent systems.

Breve Breve is a unique 3D simulation environment that focuses on decentralized systems and artificial life (Klein 2003). Like most other simulation environments, Breve is freely available.[3] The authors of Breve tout that it aims to provide a platform for physically realistic 3D models. The models simulate continuous time, and continuous space, unlike most other tool kits, which model time as discrete events and have grid world environments. In addition, some physics models, such as gravity and object collision resolution with friction, are built-in features of every simulation. Breve's OpenGL display engine

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[3]Breve website: http://www.spiderland.org/

allows for easy-to-implement 3D-accelerated graphics. Users of Breve must use a custom object-oriented language called Steve.

One of the motivating applications for building Breve was Sims' (1994) evolved 3D creatures (Klein 2003). In this project, creatures composed of several blocks and joints compete in a game to be closest to a ball. The features of Breve naturally fit to this domain, since it has physically realistic servos and objects that can interact with one another. Due to these features, Breve is an interesting system for modeling individual mobile agents, as well as multiple mobile agents.

MASON   MASON is a freely available multi-agent simulation toolkit developed at George Mason University.[4] MASON takes a different approach than previous multi-agent tool kits in that it strives to be minimalist and efficient for up to a million agents (Luke *et al.* 2005). It is meant to be run on a number of back-end computation servers in parallel, without visualization.

MASON does not have any domain-dependent tools or built-in environments like Breve or Repast, leaving the user to implement their environments in Java. Although MASON is quite minimalist, it is designed to be extensible so that it can be used as a foundation for new simulation systems.

MASON simulations can be interacted with using a separate visualization that binds to the simulation. This is a different paradigm than other tool kits like NetLogo that are tightly coupled with the visualization.

NetLogo   NetLogo is a relatively new ABM system, which was started in 1999 at of Northwestern University as a derivative of StarLogo (Tisue & Wilensky 2004). The software is free to download,[5] but not open source. As the name suggests, the language

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[4]MASON website: http://cs.gmu.edu/ eclab/projects/mason/
[5]NetLogo website: http://ccl.northwestern.edu/netlogo/

used by NetLogo is a derivative of Logo, a Lisp-like language. An artifact of this language is that agents are referred to as "turtles" in NetLogo.

NetLogo's language is tailored to the agent-based model paradigm. Particularly, a program can change context to an individual and execute code from its point of view. Also, populations of agents can execute these individual actions concurrently. For example, the code to ask all the agents to move forward one unit, then turn right would be:

```
ask turtles [ fd 1 rt 90 ]
```

Other than turtles, there is another built-in agent type: the "patch." Patches are organized as a grid in a two-dimensional environment to which agents are confined. Users can interact with patches from their context, like the turtles. Also, it is easy to retrieve turtles that are in contact with a patch and to retrieve which patch a turtle is on, from their respective contexts. This makes turtle interactions with the environment simple to implement.

NetLogo also includes a built-in user interface and user interface editor. The interface consists of controls, monitorsm and the domain visualization. Users define controls that bind to global variables and buttons that bind to function calls. In addition, users can add monitors and plots, which show a variable's value or plot a variable's value over time. These are useful tools in conveying information that the domain visualization cannot. NetLogo can be run "headless" to facilitate parallel execution of models or to reduce run-time.

NetLogo comes with a number of extensions, most notably BehaviorSpace and Hub-Net. BehaviorSpace is a tool for designing a series of systematic experiments with different system configuration parameters. BehaviorSpace performs a user-defined measurement value after each individual execution and reports the result to a data set in the form of a spreadsheet. HubNet is a server/client tool that allows several users of a system to interact with a NetLogo ABM at the same time, which is useful for classroom instruction.

NetLogo can be interacted with from an external Java API. A NetLogo "workspace"

is instantiated as an object and can be used to send commands and to query current variable values. This capability is useful for an number of tasks. First, sometimes NetLogo's language is not expressive enough and some may find programming in Java more familiar. In addition, external Java libraries (such as machine learning libraries) can be used without modification by integrating with NetLogo from its Java API. Also, a sequential experiment system can be implemented in Java if a user would like to run experiments without BehaviorSpace.

An extensive model library with over 140 sample models is bundled with the NetLogo distribution. These already existing models serve as excellent examples for new models as well as starting points for modified models. Most of the domains discussed later in this dissertation are from this model library.

NetLogo is my ABM system of choice for this dissertation research for a number of reasons. First, NetLogo's learning curve is surprisingly short. From personal experience, an experienced programmer can learn to write a domain similar to the Wolf Sheep Predation model in less than an hour. In addition, the documentation[6] is well organized and detailed. Second, the model library provides several models that are interesting and easy to work with. Since each of these models are implemented in NetLogo, I was able to implement AMF so that it interacts with each ABM in a similar way. Other multi-agent system toolkits provide more flexibility in implementation, which would make identifying agent-level control parameters and system-level properties more difficult. Third, although NetLogo's platform is well contained, the interactions possible with the Java API make almost anything possible. I was able to implement my framework as an external modular application that interfaces with NetLogo, instead of as a built-in system-dependent tool. This property makes my research easily extensible to other ABM systems in the future.

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[6]The NetLogo documentation is available at http://ccl.northwestern.edu/netlogo/docs/

3.2 Regression

Regression is an integral part of this dissertation research, as it provides the foundation for solving the forward- and reverse-mapping problems. Regression techniques are used to predict values of dependent variables, given values of the independent variables. The typical approach is to use a model developed from a sample training set to infer new values that of configurations that have not been sampled. Also, regression can be used to smooth the natural error in sampling.

Linear regression is perhaps the simplest form of regression. It fits a line to represent the correlation between one independent variable and one dependent variable, taking the form of:

$$y = x + b.$$

There exists a closed-form solution to determine m and b in order to minimize the sum of squares between the training data and the curve.

Unfortunately, linear regression is limited in that it only models linear relationships, and is not able to model nonlinear ones, such as rhythmic oscillations or quadratic correlations. Two paths are generally taken to address this concern. The first is to use the kernel trick (Muller *et al.* 2001) to map nonlinear data to be linear, but higher-dimensional. Then, once the data is projected into a space in which it is linear, linear methods (e.g., linear regression, perceptrons (Minsky & Papert), or support vector regression (Smola & Schölkopf 2004)) can be used.

The second approach is to use nonlinear methods, which relax linear regression to learning a function $f : \mathbb{R}^n \to \mathbb{R}$ that satisfies the following equality:

$$y_i = f(\mathbf{x}_i) + \varepsilon_i.$$

In this equation, y_i is a dependent variable and $\mathbf{x}_i$ is the vector of independent variables associated with y_i. Also, there is an assumption of some normally distributed and independent error with each point, denoted by ε_i. The process of *nonparametric* regression is to estimate this function directly (Fox 2002).

Alternatively, a *parametric* regression model keeps the form of the function $f(\cdot)$ fixed, but changes parameters to this function, instead. Instead of learning $f(\cdot)$ directly, a vector of model parameters β are optimized to fit the data (Fox 2002):

$$y_i = f(\beta, \mathbf{x}) + \varepsilon_i.$$

For example, $f(\cdot)$ could model two-dimensional sinusoidal data with the model:

$$f(\beta, (x_1, x_2)) = \beta_1 + \beta_2 \sin(x_1 - \beta_3) + \beta_4 \sin(x_2 - \beta_5)$$

Typically, the value of the least squares metric is minimized to fit the curve to the data.

While developing the ABM Meta-modeling Framework, I needed regression algorithms that satisfied a number of properties. The regression algorithm should scale well with dimensionality, since agent-based model behavior spaces (i.e., the space of agent-level parameters and system-level properties) are typically high-dimensional. I also needed algorithms that could model nonlinear correlations, since behavior spaces are diverse and rarely maintain linearity throughout the entire space. However, in the ABMs I have experimented with, all spaces are very smooth locally. That is, there is little variance in values between nearby locations in the behavior space. Even in the situation where there is variance, the error is typically evenly distributed and cancels out if the same configuration is sampled a number of times. Therefore, nonlinear parametric regression can fit to the overall behavior space, without having to worry about fine-grained variations in the data. Also,

the mappings built by the regression models should be smooth. This smoothness property is important for the tractability of finding the reverse mapping, since bumpy surfaces will naturally yield more intersections than smooth ones. Therefore, regression methods that smooth the data, such as LOESS, are effective in this situation.

In the course of testing AMF, I used three regression techniques: k-nearest neighbor, LOESS, least-squares nonlinear regression.

3.2.1   K-Nearest Neighbor Regression

K-nearest neighbor (KNN), in general, is the process of selecting the k nearest points to some point $\mathbf{x}$. These points can then be used for classification or regression. In the simplest case, each neighbor's y value is averaged to infer a value $\hat{y}$ for the given point $\mathbf{x}$. KNN is easy to implement and accurate with large data sets. The accuracy of this regression can be improved by weighting points by distance or by using a secondary regression algorithm (e.g., linear regression) on the neighbors.

We use KNN in our results as a baseline, since it is easy to implement and accurate. In addition, it is nonparametric, which makes it agnostic to the shape of the behavior space. Therefore, KNN requires little to no configuration or tailoring to a particular domain.

However, when implemented naively, the running-time scales linearly with the size of the data set because the process of finding the nearest neighbors requires a scan of all data points. This search time can be reduced with the implementation of faster searching techniques, such as locality-sensitive hashing (Gionis, Indyk, & Motwani 1999), among other methods. Even with faster neighbor-locating techniques, some sort of search is required for each query to KNN.

Selecting k is an important step, as different values of k will fit the data better than others. If k is too low, the regression will be overfit since it is ignoring many of the points. If k is too large, the regression will be overgeneralized and provide a mapping that is too

smooth. Unfortunately, the nature of the data and the size of the data set determine which k is best. To determine a proper k, I use the standard technique of using 10-fold validation to determine which in a set of candidate k values results in the least average error.

The spaces generated by KNN are not continuous (particularly if the neighbors are not weighted). This is because similar points will have the same neighbors and, in effect, have the same predicted value. There are inflection points one side of where the k-nearest neighbors will include a particular data point, whereas on the other side it will not. At this separation, there will be a discontinuity in predicted values. This can be a problem for solving the reverse-mapping problem because the intersection between hyperplanes generated by KNN will not intersect smoothly. This can be remedied by using KNN in conjunction with multilinear interpolation.

3.2.2   Robust Locally Weighted Regression and Smoothing Scatterplots (LOESS)

Robust Locally Weighted Regression and Smoothing Scatterplots (LOESS) is a mature nonparametric regression technique for fitting curves to data (Cleveland 1979; Cleveland & Devlin 1988). Similar to k-nearest neighbor, LOESS uses local points to infer values of new data points. LOESS also iteratively smooths the regression curve, allowing for variable magnitudes of smoothing. This is important for particularly noisy data sets. The role of LOESS in the testing of AMF is that it is more robust than KNN, yet still nonparametric.

Abstractly, LOESS fits a new $\hat{y}_i$ to every $\mathbf{x}_i$ to replace the original noisy y_i. Then, LOESS iteratively smooths each $\hat{y}_i$ to reduce variability. Specifically, LOESS follows the following steps:

1. Initialization step – For each $\mathbf{x}_i$, weight all other points x_j, where $j = 1...n$, based on a weighting function $W(\mathbf{x}_i, \mathbf{x}_j)$. which weights closer points higher. Perform

weighted linear regression to infer $\hat{y}_i$.

2. Smoothing step – For each $\mathbf{x}_i$, weight all other points based on w_i, as well as a new weight function δ, which returns a magnitude inversely proportional to $y_i - \hat{y}_i$ (i.e., the larger the distance, the lesser the weight). Perform weighted linear regression to infer $\hat{y}_i'$.

3. Set each $\hat{y}_i$ to $\hat{y}_i'$.

4. Repeat the the smoothing step as many times as necessary.

Values in between $\mathbf{x}$s can be now be interpolated.

LOESS can be customized in a number of ways. The different weighting functions can be changed to change the amount of influence that other points have on the linear regression step. Typically, these weighting functions have a "smoothing" parameter, which increases the influence of further away points, effectively reducing the strong influence of local points. Adjusting the smoothing parameter is important because if it is too low, the regression curve will be erratic (i.e., overfit), whereas, if the smoothing parameter is too high, some features of the curve may be eliminated.

LOESS is computationally expensive in comparison to other approaches, because weights are applied and points are readjusted iteratively a number of times. However, the model can be built offline and then stored. Once the $\hat{y}_i$ values are inferred, they can be used to interpolate new points (similar to multilinear regression) in response to queries. Caching these values provides a quick response time to users wanting to infer $\hat{y}$ values. This property satisfies one of the design criteria of AMF: the regression algorithm should be fast for the user.

3.2.3   Nonlinear Regression

Nonlinear regression (NLR) is a parametric approach to regression. In this approach, a parametric model is provided by the user that represents the relationships in the data, in general. This is typically done based on some sort of intuition provided by the user. For example, the data may appear sinusoidal or quadratic, in which case a model involving sine curves or quadratic polynomials, respectively, would be appropriate. Similarly to how linear regression will not model nonlinear relationships well, certain nonlinear models will not model other nonlinear relationships. Therefore, accuracy is largely dependent on the selection of the correct model.

Optimization techniques, such as Gauss-Newton or Levenberg-Marquardt (Mor 1977), are used to adjust nonlinear model parameters in order to minimize the least squares metric (Gallant 1975). These processes iteratively move models towards the best fit to the data.

Nonlinear regression is of particular interest in my research because it is analytically invertible, since trained NLR models are already in the form of a function. Unfortunately, since NLR is parametric, it requires a significant amount of configuration for each target domain.

Chapter 4

DEFINING SYSTEM-LEVEL PROPERTIES

System-level properties play a central role in this dissertation. A system-level property is a mathematical measurement of some non-explicit concept of interest in an agent-based model. These properties are typically non-explicit, and dependent in complex ways on the explicit parameters, which means that inferring their values from just the given agent-level configuration parameters is difficult.

Identifying which system-level properties of an ABM to analyze is the first step of using the ABM Meta-modeling Framework. Deciding which features should be measured is a task for the user of the framework and will be influenced by what that user finds interesting or what that user needs to analyzed. Each system-level parameter is defined as a mathematical measurement of the behavior in terms of observable features of the ABM. For example, the average number of sheep in the Wolf Sheep Predation model is a system-level property of the system that is calculated by averaging the number of sheep measured in each time step over the lifetime of the system. The framework utilizes the user-provided mathematical definition to create a data set that is used in the forward mapping.

In this chapter, I discuss the problem of defining system-level properties for use in AMF. First, the important "stability assumption" and the consequences of this assumption are explained. Next, a comprehensive list of common system-level property classes is

outlined. This list should be useful for users of AMF in defining their own system-level properties. Then, the process in which AMF uses to sample an ABM is explained. Finally, software implementation details are given for this particular step of AMF.

4.1 The Stability Assumption

Before delving into the topic of defining system-level properties, I first discuss the "stability assumption." Understanding this assumption and its consequences is important in defining system-level properties so that they will be measured accurately by AMF.

AMF assumes that the naturally occurring error for sampled values of a system-level property must have the following feature: the expected mean and expected median of the behaviors should be identical. In other words, the errors should be expected to be evenly distributed around some value $\bar{y}$, in both magnitude and quantity. Errors following a normal distribution will have this property. For example, the percentage of trees burned down in the Fires[1] model will vary from run to run, but for the most part will be centered around one value for a particular configuration.

If this assumption does not hold, regression algorithms will bias their predictions. As more points are sampled, the regression algorithm's predictions will converge on the value provided by the mean of measured values. However, the median may be a better predictor of the expected behavior if the errors are not normally distributed. This problem is best explained with an example.

In the Wolf Sheep Predation domain, a simple system-level measurement is the average number of wolves after a thousand time steps. This number can be misleading, because certain configurations will *sometimes* result in the wolves going extinct (i.e., zero wolves). Other times, the same configurations will result in the wolves converging to a stable non-

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[1]The Fires model is discussed in more detail in Section 5.1.

zero population. When the wolf population does stabilize, it generally converges upon the same population value, $\bar{w}$. However, the average of successive runs will result in a bimodal distribution, with a single spike at zero and a tight distribution of values around this stable population size, as shown in Figure 4.1. Unfortunately, this average is not useful in any way, since it does not tell how often the wolves will go extinct or what their population will be, should it be the case that the population stabilizes.

To remedy this problem, the population measure can be decomposed into two components: the average populations in the case where the wolves become extinct and the case when they do not. The average number of wolves $\bar{w}$ can be then be posed as:

$$\bar{w} = \mathrm{P}(extinct) * (\bar{w}|extinct) + (1 - \mathrm{P}(extinct)) * (\bar{w}|\neg extinct)$$

where $extinct$ is true when the wolves became extinct, $\mathrm{P}(extinct)$ is the probability that the wolves become extinct, and $(\bar{w}|\neg extinct)$ is the average number of wolves, given that they do not become extinct. The value of $(\bar{w}|extinct)$ is zero, so the left hand side of the above equation is zero. Therefore, the equation can be simplified to:

$$\bar{w} = (1 - \mathrm{P}(extinct)) * (\bar{w}|\neg extinct)$$

As stated earlier, $\bar{w}$ is biased because in some cases an experiment will return zero and sometimes it will return $(\bar{w}|\neg extinct)$. However, the values $\mathrm{P}(extinct)$ and $(\bar{w}|\neg extinct)$ are useful in describing the system's behavior and are more stable (and accurate) than just using $\bar{w}$. The system-level properties that should be measured for the Wolf Sheep Predation model are not the average number of wolves, but the average number of wolves given that they did not go extinct, and the probability of the wolves going extinct.

To calculate the value of $\mathrm{P}(extinct)$, one can divide the number of samples that ex-

hibited zero wolves by the number of total samples for that configuration. To calculate the value of $(\bar{w}|\neg extinct)$, one can average the population size of the wolves in the samples in which they did not go extinct.

The histogram in Figure 4.1 illustrates why $\bar{w}$ is a poor metric for this domain. I measured the average number of wolves post-convergence in 850 runs of the same configuration[2] of the Wolf Sheep Predation model. In this experiment, 303 of the 850 samples resulted in the wolves going extinct. The other 547 samples had their wolf populations stabilize. The average number of wolves over all samples $\bar{w}$ is 44.69. The value 44.69 has little meaning in this domain, since it does not tell us about the stable wolf population size, or how often the system will exhibit zero wolves. In fact, the actual number of wolves is *never* close to $\bar{w}$. The estimated probability of extinction is $P(extinct) \approx 303/850 \approx .356$. The average number of wolves in a stable population is $(\bar{w}|\neg extinct) = \sum(w_i)/547 \approx 69.45$. These two values explain the the behavior of this particular Wolf Sheep Predation model instance more accurately than $\bar{w}$.

In many situations, non-stable system-level properties are the result of some sort of *threshold effect*. Threshold effects are sudden changes in behavior, given a small change in the configuration. Threshold effects are also sometimes referred to as *tipping points*. In ABMs that incorporate random behavior, configurations that are on a boundary of a threshold effect can exhibit erratic behavior,as in the Wolf Sheep Predation example. Typically, this problem can be overcome by decomposing the property into several sub-properties that describe the threshold effect. This approach is what was needed to provide useful and accurate information in the Wolf Sheep Predation example.

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[2]The parameters were grass-regrowth-time = 22, initial-number-sheep = 100, initial-number-wolves = 50, sheep-gain-from-food = 4.7, wolf-gain-from-food = 20, sheep-reproduce = 3%, wolf-reproduce = 4%.

Histogram: Number of Wolves
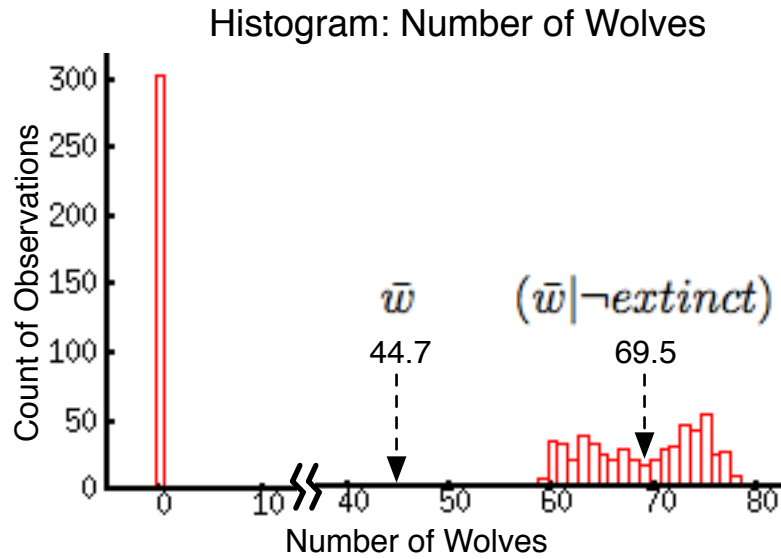
FIG. 4.1. A histogram of the number of wolves after many successive runs shows that the average number of wolves is a poor measure the system behavior.

4.2 Common Classes of System-Level Properties

Through the course of identifying a number of system-level properties in a variety of domains, I have found that most properties fit into one of these general classes.

4.2.1 Average of a Value

One of the simplest measurements is the average value of a property over the life of the system, which is useful for measuring behavior that converges over time. To measure this property, the property is measured every time step up until a predetermined stopping point, and then averaged.

A few modifications to this simple approach are possible. First, the recording of values can be delayed for a number of time steps to allow the system to converge. If convergence is ignored, the values recorded before convergence may bias the results in an unexpected way. To remedy this, only the points post-convergence are used for the average. The next
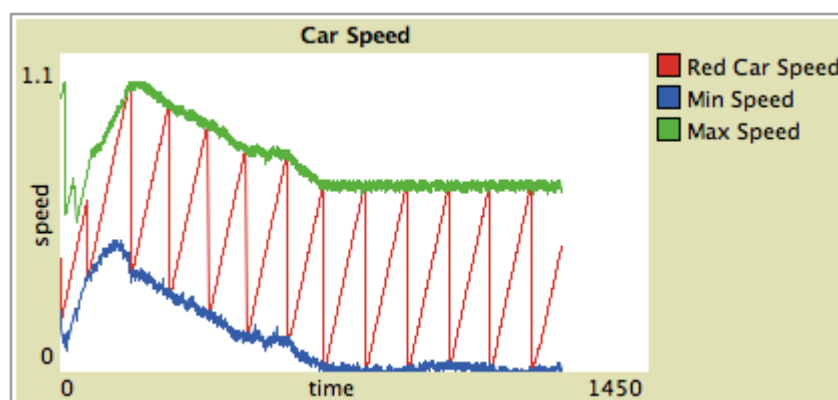
FIG. 4.2. The behavior of the NetLogo Traffic Basic ABM converging after about 650 time steps.

step is to determine what this "post-convergence" happens. The simplest method is to determine a duration of time in which most model will have converged. Another naive method is to just sample for a very long time. As time passes, the average will converge to the convergent value, since more values representing the convergent behavior will factor into the average. A more advanced technique would be to detect when the system values have stopped changing significantly and start measuring from there.

In Figure 4.2 (a plot from the NetLogo Traffic Basic ABM), the maximum speed and minimum speed of the vehicles converge to .65 and 0, respectively. However, before time step 650, the behavior was quite different than the eventual convergent behavior. If each time step (0 to 1250) were averaged, the maximum speed value would be biased to be larger than .65. This number has some meaning, but not the "average top speed" that was expected. The average should be comprised of values after time step 650 to match the actual measurement with the expectations.

This class of measurement should not be used on properties that diverge (i.e., fail to converge on a single value over time). In divergent cases, the average will continue to increase or decrease as more time steps are used in the measurement. Instead, the aver-

age value should converges as more time steps are measured. The value produced by the forward and reverse mappings will be inaccurate and meaningless if this property does not hold because the value would be dependent on how many time steps the system was sampled, and would have very little to do with the value of the behavior itself.

4.2.2 Variance of a Value

The variance of a value over the life of a system is a useful metric for determining how "stable" the property is. If the property changes significantly from one time step to another, the variance will be higher than that of a property in which the value remains stable. Figure 4.3 shows a comparison between two situations in which the variance of values are different.

(a)   (b)
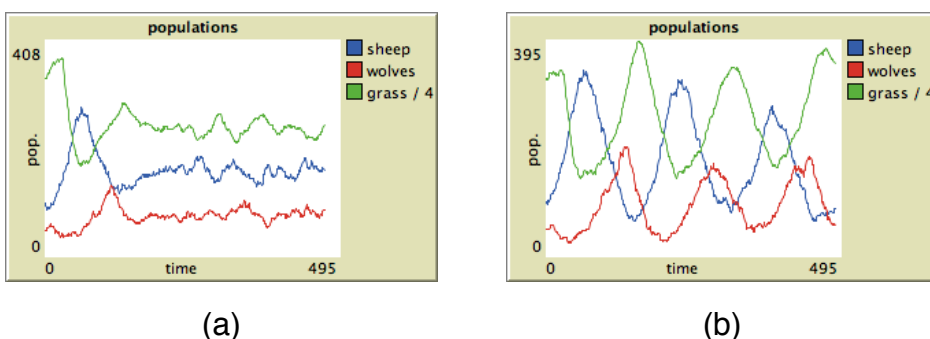
FIG. 4.3. Two different behaviors in the NetLogo Wolf Sheep Predation ABM with similar average sheep, wolves, and grass values. The two can be distinguished by the variance: the values in (a) have a lower variance than the ones in (b).

Similar to averaging system-level properties over time, only values after convergence should be used to calculate the variance. This must be done to avoid biasing the variance of the behavior after it has converged. Taking this problem into consideration is particularly important in this for the variance metric because systems' behaviors typically vary significantly before convergence.

Also similar to the average value metric, this variance metric should not be used on behaviors that diverge. As a divergent property value continues to increase or decrease, the variance will increase. The variance converges on a single value as more time steps are sampled, for the same reasons that the average metric should converge.

4.2.3 Probability of a Threshold Effect

Threshold effects are binary properties that may or may not appear in a run of a system. These tipping points divide the behavior space into configurations that exhibit the threshold effect and ones that do not. Configurations near the threshold will often vary in which behavior side of the threshold they will converge to. For example, in the Wolf Sheep Predation ABM, wolves may or may not be extinct when the system converges. With some configurations, the wolves will always go extinct, but in others the wolves never go extinct. Configurations on the boundary between wolves going extinct and not will exhibit both of these outcomes in different runs, due to the inherent randomness in the system.

One particularly useful metric for analyzing threshold effects is the probability that a certain configuration will exhibit the threshold effect. For example, in the Wolf Sheep Predation ABM, a system-level property could represent the probability that the configuration will result in the wolves going extinct. To measure this property, several experiments need to be executed for a single configuration. The probability is estimated by calculating the proportion of iterations that had no wolves, to the total number of experiments. The value of this probability should converge as more experiments for a single configuration are executed.

4.2.4 Measuring a Value That Changes Over Time

The previous measurements assume that the behavior will converge over time, which is not the case for all behaviors. Also, there are situations in which the average value or

the variance of a value does not convey enough information. In particular, properties that change over time may not fit into the above classes.

So far, all properties have been scalar values. The framework works only with scalar values and is unable to naturally predict how a behavior will change over time. To circumvent this issue, the system-level properties could be parameters of a parametric model that represents a behavior that changes over time. Predicting each behavior is essentially a nonlinear regression problem, in which the independent variable is time and the dependent variable is the property.

The parameters of the behavior's parametric model are learned in the forward mapping process as individual prediction problems: N different forward mappings will be learned for each of the N parameters. The value for each parameter is predicted by the corresponding mapping, given the system's agent-level configuration. These predicted parameters can be plugged into the parametric model to generate a curve that represents the behavior over time.

This approach can be applied to a number of phenomena, such as the ones illustrated in Figure 4.4. In Figure 4.4(a), the animal populations in the Wolf Sheep Predation model vary rhythmically and could be modeled with sine curves. The parameters of these behaviors modify the magnitude, height, and frequency of the sine curves. In Figure 4.4(b) (a plot from the NetLogo AIDS model (Wilensky 1997a)), the *HIV-* (people without HIV) curve decreases and *HIV+* increases in a sigmoid pattern. The parameters of these two sigmoid behaviors modify the shape of the sigmoid function. The *HIV?* (people who have HIV but do not know it) value appears to follow a curve that is similar to a probability distribution. However, it is simpler to model this property in terms of the other two: the HIV- and HIV+ values subtracted from the total population. In Figure 4.4(c) (a plot from the NetLogo Firebugs model (Wilensky 1997b)), the behavior converges to zero over time. The rate of convergence (i.e., the slope of the curve) would be the parameter for the model of this
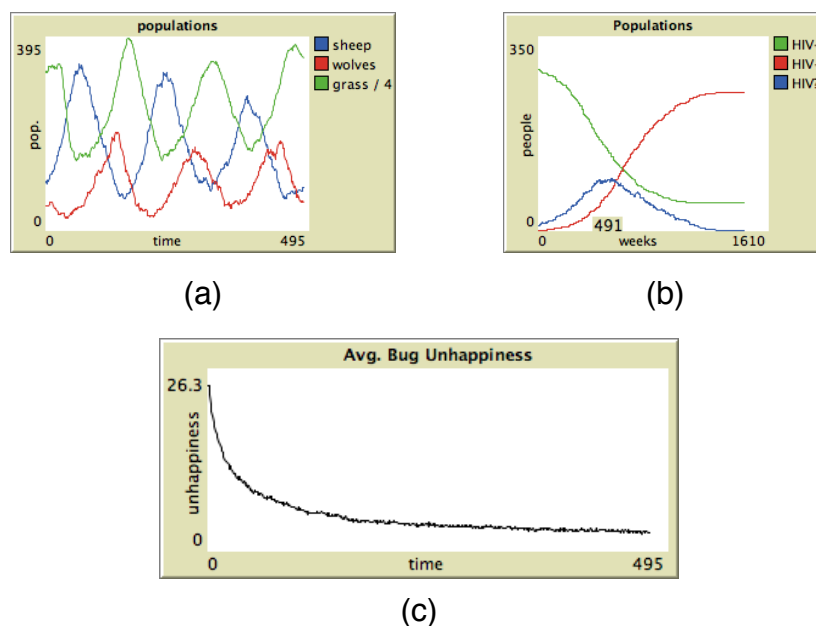
FIG. 4.4. Different types of behaviors that change over time in NetLogo ABMs.

behavior. This general approach is applicable to any property that can be described by a parametric regression model.

These system parameters are measured during sampling by performing parametric nonlinear regression for each experiment to determine good values of the parameters. These parameters are the system-level properties for AMF, but can be interpreted by the user as the parameters to the regression model.

Custom models can be developed for particular domains. Consider the NetLogo Traffic Simple simulation, in which cars move in a single lane. Traffic jams appear in waves, which is illustrated by the speed of the red car,[3] as illustrated in Figure 4.2. We would like to develop a mapping to represent the velocity of the red car. From visual observation, it appears that the red car has a constant minimum speed and a maximum speed. It is known

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[3]Nothing is special about the red car in the Traffic Simple situation. It is singled out to show the traffic pattern from the perspective of an individual.

that the acceleration is linear from the programming of the model. Also, the red car follows a rhythmic behavior: the car reaches a certain speed, then stops. With these observations, the information necessary create a wave-like parametric model that describes this behavior is available. The following variables are used in the parametric wave model:

- Let A be the amplitude of the wave (i.e., the maximum velocity minus the minimum velocity).

- Let T be the period of the wave (i.e., the time between the occurrence of a maximum velocity and the occurrence of a minimum velocity).

- Let h be the height of the wave (i.e., the minimum speed).

The behavior within each period is linear, so it can be described as a simple linear model:

$$speed(t) = \frac{A}{T} t + h.$$

Since this behavior is periodic, modulus T is used to reset the behavior back to the minimum spread.

$$speed(t) = \frac{A}{T} (t \bmod T) + h.$$

The forward-mapping problem would involve predicting values for A, T, and h, given the configuration of the system. For each experiment, nonlinear regression is used to find good values for A, T, and h, which are recorded as the dependent variables.

4.3 Sampling

The sampling process may begin once the system-level properties are defined. The AMF sampling process consists of two major steps: (1) retrieve raw data (i.e., observed agent behaviors each time step) from the simulation; and (2) use that data to compute the

values of the system-level properties (e.g., average and variance of specific behaviors). Instead of performing the calculations while sampling, I prefer a method of computing the actual statistics from a raw data set. This process permits new statistics to be measured using the raw data at a later point in time without having to re-sample the system.

The AMF uses an evenly distributed random sampling technique. Ranges for parameters are passed to the sampling program and random values within these ranges are generated for each experimental configuration. This technique is flexible because it allows the side of the data set to be changed dynamically for testing purposes. Also, new points can be sampled to increase the accuracy of the data set in a particular area. The initial regression algorithms I have selected to assume AMF work with randomly distributed data. More advanced sampling techniques could be used in future work.

Sampling the same point repeatedly, instead of generating a new point per experiment, has several uses. Different samplings of the same point could be used to:

- Measure the variance of a variable between samples to determine its stability,

- Determine the probability of a threshold effect being exhibited,

- Smooth the data set by reducing natural error, or

- Generate more accurate individual points.

For these reasons, I typically sample each randomly selected point several times, instead of sampling a wider variety of points once.

4.4   Implementation Details

The AMF implementation for defining system-level properties and performing sampling is designed to require a minimal amount of user programming. The sampling process consists of four distinct steps:

1. Identify, by name, which NetLogo properties need to be extracted from the simulation in order to calculate the system-level properties, and specify how often (i.e., time steps passed) each property should be measured.

2. Specify all ABM configuration parameters by name, along with the minimum and maximum values that random configurations will lie within.

3. Run the sampling application to generate the raw data set.

4. Pass the raw data set through the map[4] program, which converts the raw entries into a more compact data set that contains the desired system-level behaviors and relevant configuration parameters.

The sampling program is written in Java so that it can interface with NetLogo's Java API, which is used to run the ABMs. All of the user provided information is passed to this program in a text configuration file. A program that generates values in an identical format to the default sampling program could replace the default sampling program. Replacing the default sampling program would be useful for taking more control of the sampling process; for instance, to implement an advanced sampling strategy.

The sampling program prints the raw data to the standard output (stdout). The data is tab-delimited to separate items within entries; each entry is delimited by a newline. The entries are recorded in the order specified in the configuration file, so the configuration file can be used to give each column an identifiable name. The standard output could be redirected to store data in a file or piped to the next step.

In the final step of sampling, the "map" Python program is used to parse the raw data and output a data set that contains the system-level properties. The map script parses the data for each entry and returns aggregate or expanded statistics, per row. The output of the

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[4]The name "map" is to signify similarity to LISP's map function.

map function is then passed to the forward-mapping problem solver, which is covered in the next chapter.

Chapter 5

APPLICATION DOMAINS

Four target domains are used to demonstrate AMF in action, showing the effectiveness of AMF in a variety of different situations. In Chapter 8, experiments are performed on each of these ABMs to evaluate AMF. No modifications to AMF have to be performed to make AMF compatible with these domains, which shows that AMF is domain-independent. In each of the domains enumerated in this chapter, I give a brief overview of what the ABM represents, what configuration parameters are available, and what system-level properties I have defined.

5.1 NetLogo Fires

The NetLogo Fires ABM is the simplest ABM used in this dissertation. In this ABM, trees are distributed throughout a 250×250 grid world. A fire is started in the left column, after which all trees in this column burn. Each burning tree then burns its adjacent trees (up, down, left, and right). This process continues until no more trees are adjacent to burning trees.

The configuration space and the system-level property space are both one-dimensional. The configuration parameter for this domain is the density ρ of the forest, which in the experiments ranges from 45 % to 75%. This parameter changes the probability that a grid

density control

percentage of
trees burned

safe trees   burned trees
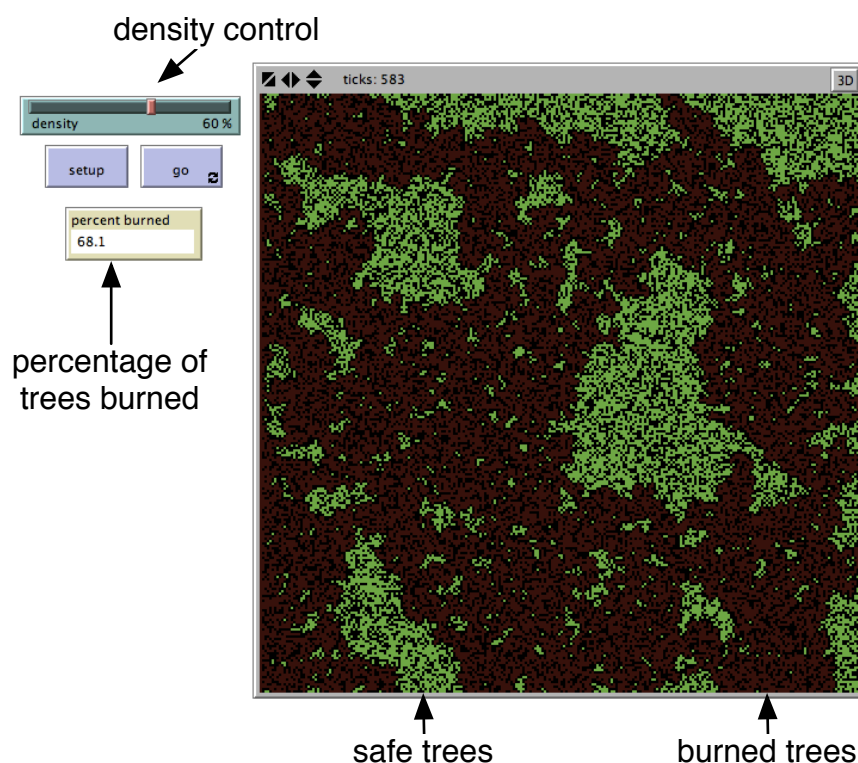
FIG. 5.1. Screen capture of the Fires NetLogo ABM.

point contains a tree: during the initialization step, each grid point has a tree placed with probability ρ. The system-level property is the percentage of trees burned down, which is measured by dividing the number of trees that were burned by the total number of trees originally in the system.

The Fires ABM is particularly interesting because it exhibits a threshold effect. There is a sharp transition from small amounts of the forest burning down to the entire forest burning down when the forest density increases past 58%. The behavior space is not linear: it exhibits high variance around 58%, making this ABM moderately challenging, despite having only a single configuration parameter.

5.2   NetLogo Flocking

The NetLogo Flocking ABM is a classic agent-based model based on rules devised by Reynolds (1987). As in the original work, the emergent flocking behavior results from the summation of the following forces:

- *avoidance* – repel agents that are too close to one another,

- *center* – attract agents towards the center of the flock,

- *align* – steer towards the average heading.
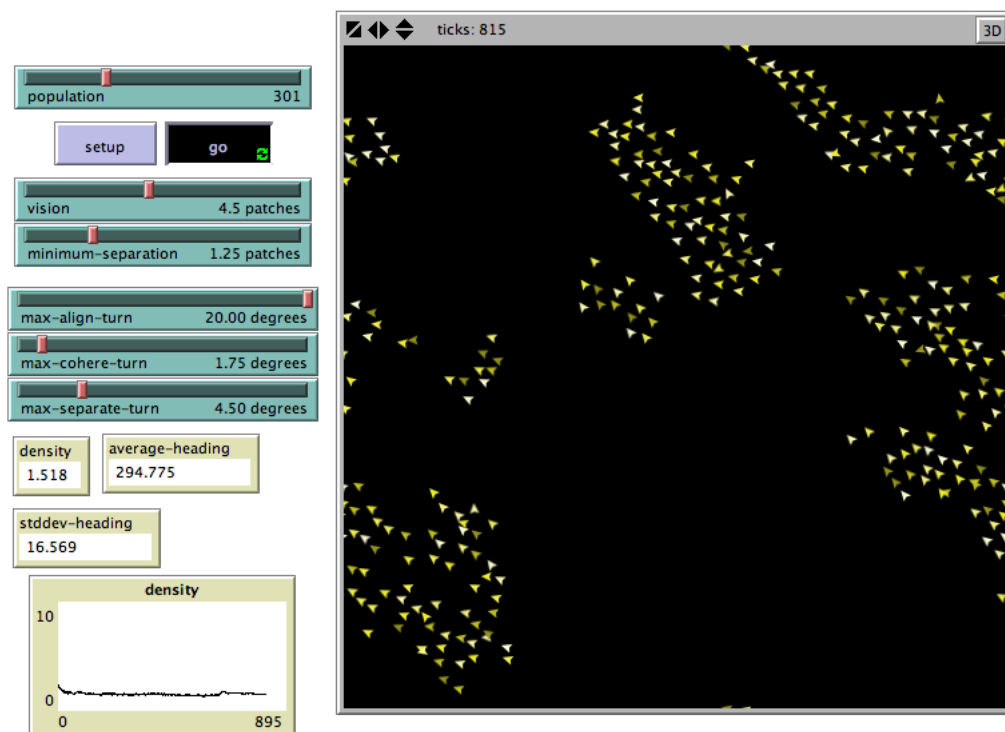
FIG. 5.2. Screen capture of the NetLogo Flocking ABM.

The NetLogo implementation of flocking follows the original definition closely. There are six configuration parameters, as seen in Figure 5.2: however, only three are used in my

experiments:

- *max-align-turn* – the maximum number of degrees an agent will turn to align its heading with its neighbors,

- *max-cohere-turn* – the maximum number of degrees an agent will turn towards the center of the flock,

- *max-separate-turn* – the maximum number of degrees an agent will turn away if another agent is within *minimum-separation*.

The other three configuration parameters available in the user interface (*population*, *vision*, and *minimum-separation*) are excluded because they do not affect the system-level properties as directly as the three outlined above. The values of these parameters are kept constant throughout the experimentation performed for this thesis.

Two system-level properties are analyzed for this system:

- *spread* – measures how spread out the agents are.

  This metric is calculated as the average distance from each agent to its nearest neighbor. This calculation is an approximation to the true density, since it does not directly measure agents per patch. Approximating is necessary because determining the area that an individual flock covers is not trivial and sometimes subjective. In addition, a single instance could have several individual flocks, making this computation even more obscure. The distance to the average neighbor captures the information that density conveys: as the distance increases, the agents are more spread out, and thus the flock is less dense.

- *stddev-heading* – measures the standard deviation of the agent headings.

  This metric is used to determine how much the agents in the ABM agree on the direction in which they are heading. Configurations with agents that flock smoothly
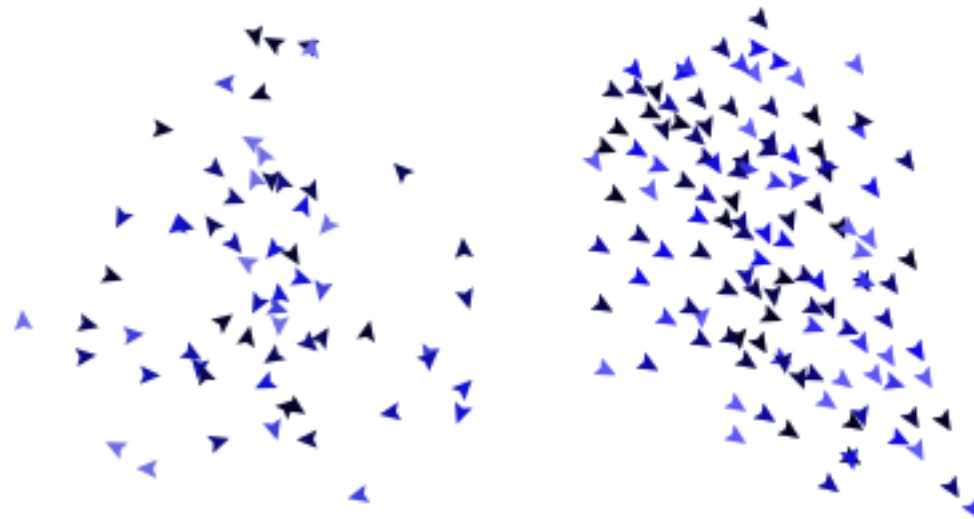
FIG. 5.3. A swarming boid system (left) and a flocking boid system (right).

in one direction have a very low *stddev-heading* value. Meanwhile, more chaotic configurations have a relatively high *stddev-heading* value, as is illustrated in Figure 5.3.

The Flocking ABM has the role in testing AMF that it is less challenging than Wolf Sheep Predation, but more complex than Fires. The system-level properties change in a more monotonic and predictable manner than the other domains, but still remains sufficiently complex. The behaviors are not linear and the configuration space is three-dimensional, making this problem nontrivial.

5.3 NetLogo AIDS

The AIDS ABM is a model of how AIDS spreads in humans. There are a number of agents in a two-dimensional world that move around randomly. Agents that collide have a chance to couple, and then have a chance to spread AIDS if one partner has AIDS (*HIV+*) and one does not (*HIV-*). Individuals that know they have the disease will not spread it to

people without it. Only individuals that have AIDS but do not know (*HIV?*) can spread the disease. Eventually, once there are no more people unknowingly spreading AIDS, the population is segregated into people who have AIDS and know it, and people that do not have it. A screen capture of the domain running in NetLogo is shown in Figure 5.4.
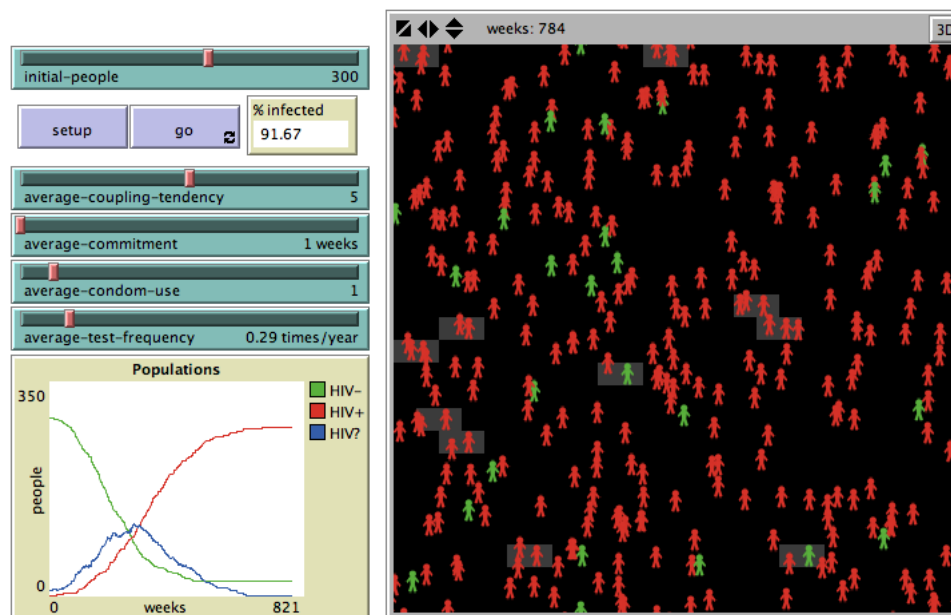
FIG. 5.4. Screen capture of the NetLogo AIDS ABM.

There are five configuration parameters available in the NetLogo implementation of this ABM. However, only two are used for the purposes of this dissertation:

- *average-condom-use* – The probability that one of the two individuals will insist on using a condom.

  The usage of a condom prevents the spread of the disease. Therefore, when this value is lower, the disease will spread to more people. When this value is higher, the opposite happens. The difference between a high value and a low value is illustrated in Figure 5.5.
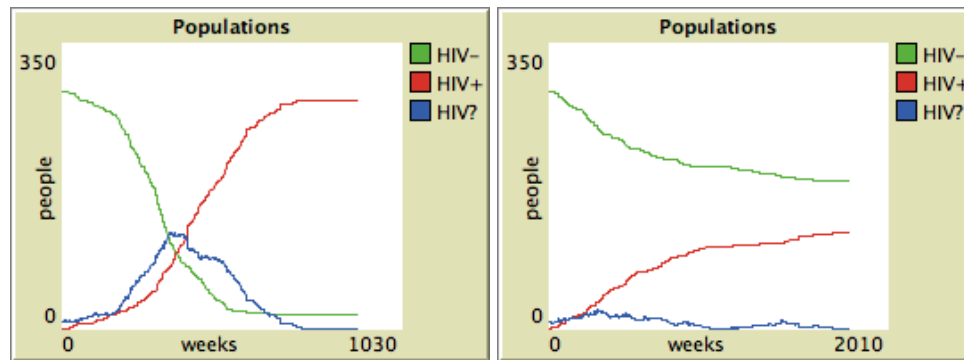
FIG. 5.5. Plot of a AIDS ABM run with low (left) and high (right) *average-condom-use* (notice the difference in the scale of weeks).
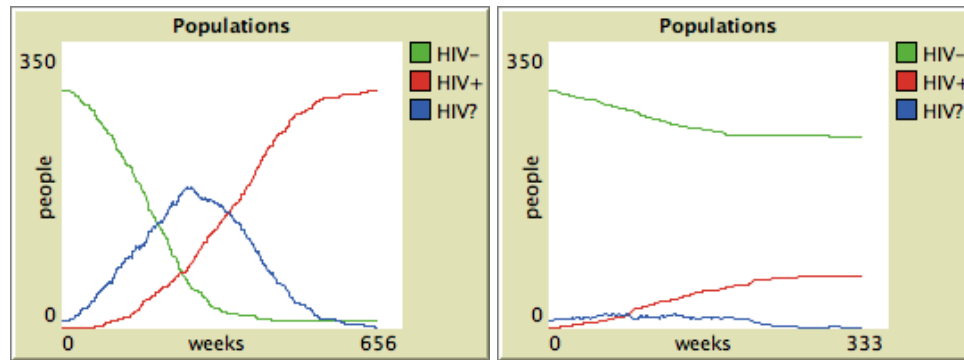
FIG. 5.6. Plot of a AIDS ABM run with low (left) and high (right) *average-test-frequency* (notice the difference in the scale of weeks).

- *average-test-frequency* – The frequency that an individual will get tested for AIDS, per year.

  Getting tested decreases the population of the individuals that have AIDS but do not know it, directly reducing the number of agents capable of spreading the disease. This parameter has a similar effect as *average-condom-use*, as seen in Figure 5.6.

The other parameters—*initial-people*, *average-coupling-tendency* (chance a couple will form), and *average-commitment* (how long a couple stays together)—are not used. I chose not to incorporate these in my experiments because they change the system-level behavior in a similar way to the two parameters that I do use. In addition, condom usage and test

frequency may be more easily affected by public policy than coupling tendency and how long a couple are committed for. Testing these real-world hypotheses are something AMF could bse used for.

The AIDS domain is used specifically to demonstrate the use of parametric models to describe system-level behaviors over time. For this domain, I will use AMF to model the plots of the populations, such as the ones in Figures 5.5 and 5.6. Nonlinear regression is used to perform curve fitting on representative parametric models, using training instances to learn the parameters. Thus, the forward mapping maps the two configuration parameters to predicted values of the parameters of the model. The appearance of the plots can then be predicted with the forward mapping.

A base parametric model that can fit the data well is required. For this domain, the curves appear to be sigmoid functions, so I will use a generalized logistic function:

$$P(t) = c_1 + \frac{c_2 - c_1}{1 + e^{-c_3(t-c_4)}}.$$

The parameters represent the following:

- c_1 – the lesser asymptote,

- c_2 – the greater asymptote,

- c_3 – the growth rate, and

- c_4 – the location of the inflection point.

The step of performing the nonlinear regression to model the curve is done after the raw data sampling and before solving the forward mapping. Each instance of scatter plot data has nonlinear regression applied to it to determine the four parameters of the logistic function. The parameters are used as the new data set, instead of the original scatter plot data.

5.4 NetLogo Wolf Sheep Predation

The NetLogo Wolf Sheep Predation ABM has been the running example throughout this dissertation. In this ABM, there are three major entities: wolves, sheep and grass. Wolves eat sheep and sheep eat grass. The grass naturally regrows; meanwhile, wolves and sheep occasionally reproduce. At every time step, sheep and wolves lose some energy and die naturally if their energy reaches zero. A screen capture of the Wolf Sheep Predation ABM in NetLogo is shown in Figure 5.7. The configuration controls are in the top left; the monitors are in the bottom left; and the visualization of the domain is on the right.
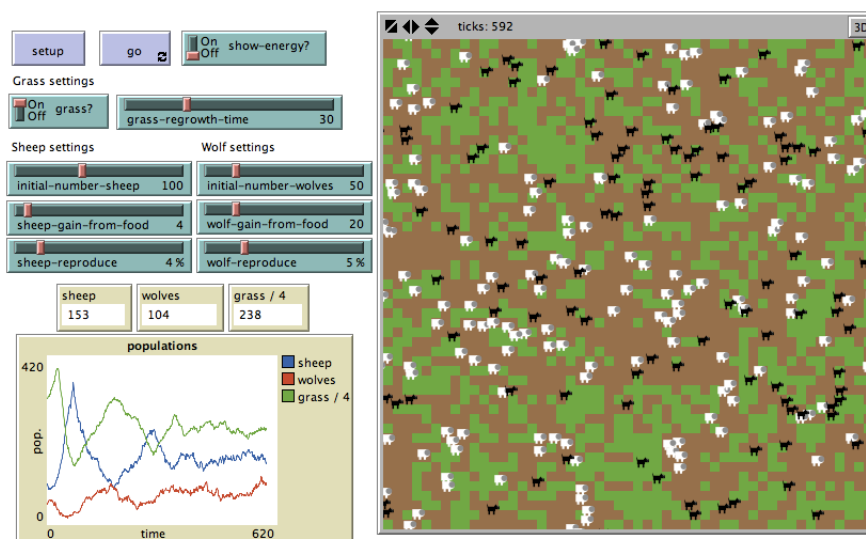
FIG. 5.7. Screen capture of the Wolf Sheep Predation ABM.

The populations of a running Wolf Sheep Predation system are constantly changing. Therefore, measuring properties is not as straightforward as in the Fires ABM. Changes in populations can range from small oscillations to high-magnitude oscillations, depending on the configuration parameters. Quantitatively capturing these properties is challenging, but is possible with AMF. A plot of a relatively normal (not too stable and not too high-magnitude) population is shown in Figure 5.8.
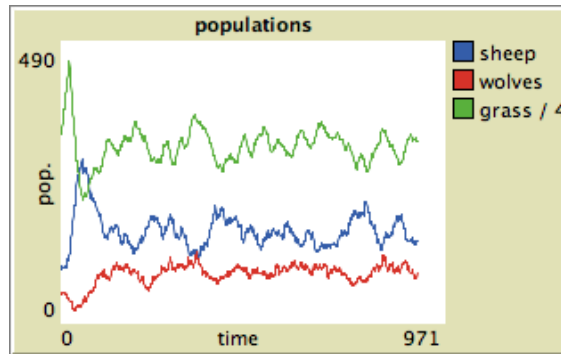
FIG. 5.8. Plot of stable populations in a Wolf Sheep Predation system.
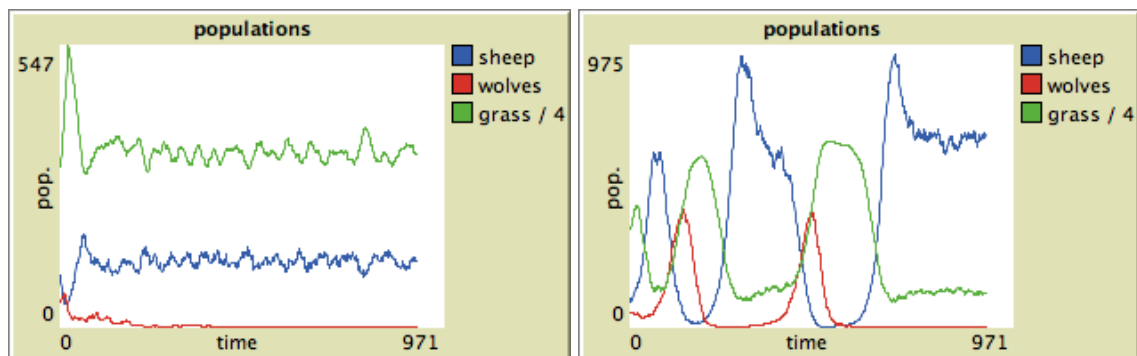
FIG. 5.9. Plot of a Wolf Sheep Predation run with low (left) and high (right)
sheep-gain-from-food.

The configuration space is five-dimensional, making this domain nontrivial to analyze. The configuration parameters, along with some general observations, are as follows:

- *sheep-gain-from-food* – the amount of energy that sheep gain from eating grass.

  This parameter has interesting effects on the system. The effect of changing this parameter from the stable norm is shown in Figure 5.9.

  At lower values, the sheep population has difficulty not going extinct, which almost always results in the wolf population also going extinct, even if the sheep eventually stabilize.

  At higher values, sheep live longer and quickly become overpopulated, which causes
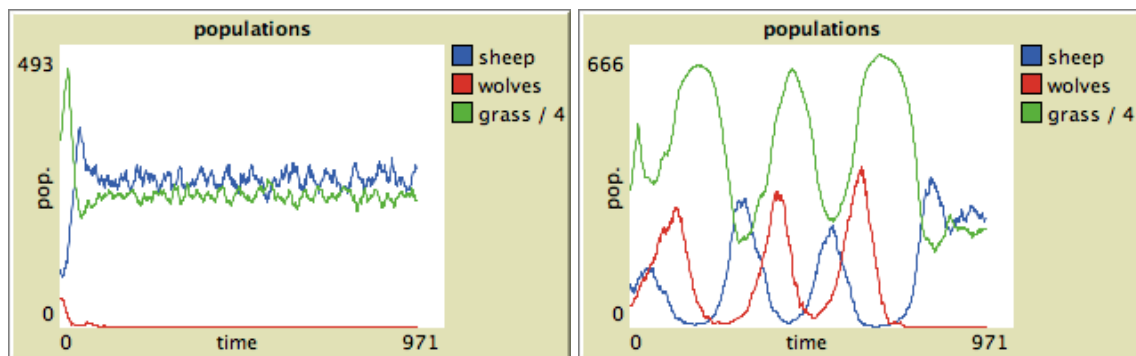
FIG. 5.10. Plot of a Wolf Sheep Predation run with low (left) and high (right)
wolf-gain-from-food.
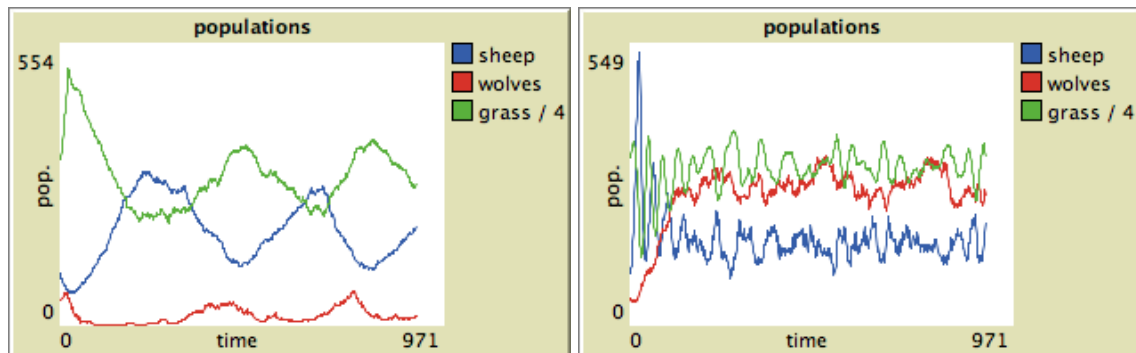
FIG. 5.11. Plot of a Wolf Sheep Predation run with low (left) and high (right)
sheep-reproduce.

the grass to become a scarce resource. With little grass left, the sheep begin to die
off. Once enough sheep have died off, the grass begins to regrow and the sheep begin
to reproduce. This results in sharp increases and decreases in sheep population as
the sheep population oscillates between overpopulated and underpopulated. When
the oscillations are of high enough magnitude, the wolves have a high chance of
becoming extinct while the sheep population is very low.

- *wolf-gain-from-food* – the amount of energy wolves gain from eating a sheep.

  This parameter affects the system in a similar way as *sheep-gain-from-food*. Lower
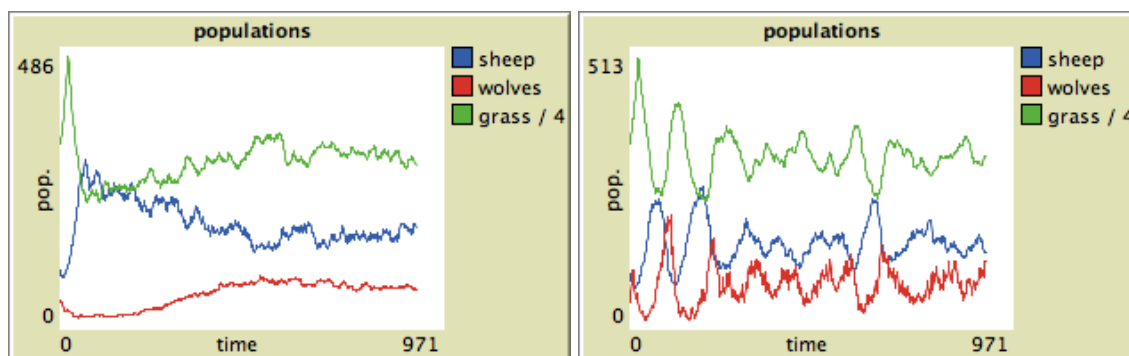
FIG. 5.12. Plot of a Wolf Sheep Predation run with low (left) and high (right)
wolf-reproduce.

values cause the wolves to go extinct, while higher values cause more dramatic os-
cillations in wolf and sheep populations. The effect of changing this parameter from
the stable norm is shown in Figure 5.10.

- *sheep-reproduce* – the probability that a sheep will reproduce, per time step.

  This parameter has the interesting property that when it is increased, the wolf popu-
  lation increases, but the sheep population remains relatively constant. When *sheep-
  reproduce* is too low, the sheep population has difficulties sustaining its numbers,
  which causes the wolf population to be very low. The effect of changing this param-
  eter from the stable norm is shown in Figure 5.11.

- *wolf-reproduce* – the probability that a wolf will reproduce, per time step.

  This parameter has relatively little effect on the system, in comparison to the other
  parameters. The populations oscillate more when the reproduction rate is higher and
  are more stable when it is lower. The effect of changing this parameter from the
  stable norm is shown in Figure 5.12.

- *grass-regrowth-time* – the number of time steps that a patch of grass takes to regrow.

This is perhaps the strangest behaving configuration parameter. At higher values, not enough grass grows to sustain a large sheep population, which causes the wolves to go extinct. At lower values, sheep rarely ever die, until they become overpopulated and eat all the grass. At this point, there is a mass extinction, which typically causes the wolves to go extinct. This parameter is similar to that of *sheep-gain-from-food* in terms of system-level behavior.

Each of these parameters individually affect the system state. Even more diverse behaviors can be observed by adjusting several parameters at once.

Several system-level properties have been developed for this domain. To sample many of these properties and to provide more consistent results, each random configuration is sampled a number of times and averaged.

- *sheep-extinct?* and *wolves-extinct?* – the probabilies that the sheep and wolf populations will reach zero, respectively.

  The probability of sheep and wolf extinction is measured by sampling the same configuration numerous times and calculating the percentage of instances in which they went extinct. Most often with a specific configuration, the sheep or wolves either always go extinct or never go extinct. However, there are borderline configurations in which the sheep or wolves will sometimes (but not always) go extinct while the system is stabilizing into a rhythm. This metric is useful in distinguishing between these three situations. Wolves will always go extinct if there are no sheep, but sheep can exist without wolves. Therefore, the value of *wolves-extinct* is always higher than *sheep-extinct?*.

- *sheep-average* and *wolf-average* – the average number of sheep and wolves, given that they did not go extinct, respectively.

The average sheep and wolf populations are calculated by averaging the populations at every time step in instances in which they did not go extinct. Not including extinct populations in the average is important because these instances will introduce significant amounts of bias. This metric describes how large the population is expected to be. Along with *sheep-variance* and *wolf-variance*, the averages describe the nature of the populations and how they change.

- *sheep-variance* and *wolf-variance* – the variance of the sheep and wolf population over the course of a run.

  The variance is calculated with the same data as the average. This metric describes how much the population changes from time step to time step, since the population is typically rhythmically changing.

The Wolf Sheep Predation ABM is interesting because its behaviors are neither linear nor monotonic. That is, as many of the configuration parameters increase, the resulting system-level behavior does not change in a linear manner. This property of the behavior space makes many of the system-level properties difficult to predict. In addition, there are five configuration parameters, which makes the configuration space five-dimensional. The system-level property space is up to six dimensions. Handling dimensionality up to eleven is a challenging task for any approach that is attempting to analyze system-level behavior.

THE FORWARD-MAPPING PROBLEM

The *forward-mapping problem* is the problem of developing a mapping from an ABM's configuration space to the user-defined system-level property space. The forward-mapping problem is the first half of building a complete meta-model of an agent-based model (the other half being the reverse-mapping problem). Learning a meta-model is made simpler by splitting the problem into two sub-problems (as opposed to directly building a bidirectional mapping from the data).

The forward mapping can be used to predict the behavior of a system without having to actually run it. This is useful because running an ABM may require too much time for hypothetical experiments. Also, in ABMs that have noisy behavior, several iterations of sampling may have to be performed to get an accurate average value. This makes sampling the original ABM even more computationally intensive. Interacting with the forward mapping is more convenient than interacting with the ABM to verify hypotheses about system-level behavior. Also, exploration of the behavior space is more efficient when interacting with a model instead of running an ABM numerous times.

This chapter details aspects of the forward-mapping problem and the solution that is used in AMF.

6.1 Definition of the Problem

The forward mapping is a functional mapping that maps *configuration space* to *system-level property space*. The configuration space is made up of the dimensions representing all the input configuration parameters of the agent-based model that could affect the system-level behavior. This space is n-dimensional, where n is the number of configuration parameters. For NetLogo ABMs, user interface elements such as sliders, text boxes, and switches provide user access to the configuration dimensions in the configuration space.

The system-level property space is made up of the dimensions representing all of the user-defined system-level properties that are being measured. Typically, these propertyies are real-valued. Since many system-level property metrics are statistical in nature, real values are used even when a discrete value is expected. For example, a expected wolf population of 70.6 still has statistical meaning, even though it is impossible to have .6 of a wolf.

The space defined by the combination of the configuration and the system-level property spaces is the *behavior space*.

An outline of the configuration and system-level property space for the Wolf Sheep Predation ABM is shown in Table 6.1. In this domain, five configuration parameters and five system-level properties are considered, so therefore the behavior space is ten-dimensional.

Let $\mathbf{y}$ be a point in system-level property space and $\mathbf{x}$ be a configuration. The forward mapping f is defined as the mapping that satisfies the following:

$$f(\mathbf{x}) \rightarrow \mathbf{y}$$

This mapping is used to answer the query "given $\mathbf{x}$, approximate the the system-level prop-

erties $\hat{\mathbf{y}}$."

$$f(\mathbf{x}) \approx \hat{\mathbf{y}}$$

Table 6.1. Outline of Wolf Sheep Predation Behavior Space

Configuration Space	
grass-regrowth-time	Number of time steps it takes for grass to regrow
sheep-gain-from-food	Energy gained by a sheep when it eats grass
wolf-gain-from-food	Energy gained by a wolf when it eats a sheep
sheep-reproduce	Probability that a sheep reproduces every time step
wolf-reproduce	Probability that a wolf reproduces every time step
System-Level Property Space	
wolf-extinction	Probability that the wolves will go extinct
wolf-population	Average wolf population, should it stabilize
sheep-population	Average number of sheep
wolf-variance	Variance of the wolf population
sheep-variance	Variance of the sheep population

A solution to the forward-mapping problem must be able to handle configuration spaces with many dimensions. Also, the methods must be able to perform accurately in both continuous and discontinuous behavior spaces. The most important aspect for any approach to solving the forward-mapping problem is that querying for a prediction must be faster than sampling the system directly and predictions should be as accurate as possible.

6.2 The AMF Approach

Regression is the default approach taken by AMF to solve the forward-mapping problem because it fits this problem naturally: the configuration parameters are the independent variables and the system-level properties are the dependent variables. The sampling phase of AMF provides a data set with measurements from numerous and diverse configurations. Each entry in the data set is a *¡configuration, system-level measurements¿* pair. These individual observations are passed to the regression algorithm as training data.

Different regression approaches use this data in different ways. Approaches like k-nearest neighbor (kNN) do not need to perform any pre-processing and instead uses the entire data set for each query. Meanwhile, parametric approaches like nonlinear regression (NLR) train a compact model, using a limited number of parameters to represent the entire data set. In general, the more time that is spent pre-processing the data, less time is spent querying. Amortized over a large number of queries, offline computation to speed up online queries is a worthwhile trade-off.

6.2.1 Scaling

Calculating the distance between two observations is an important part of many non-parametric regression techniques. Distance is used in kNN to determine which points will be factored in to determine the output value, and in LOESS to weight closer points higher (hence, the "locally-weighted" part of the name).

Different configuration parameters have different ranges and different meanings. Therefore, performing a simple Euclidean distance on these parameters to determine distances between instances will typically not yield favorable results. For example, consider *sheep-reproduce*, a percentage value in the Wolf Sheep Predation ABM, which is sampled from .01 to .08. Another parameter, *grass-regrowth*, is sampled from 5 to 30. The Euclidean distance metric treats all dimensions as equal, so closeness in the larger-ranged dimensions will be given lower weight than closeness in the smaller ranged dimension. This skew in weight can make dimensions less important, regardless of their actual importance. Properly scaling the data set rectifies this problem.

Simply scaling each dimension linearly such that the minimum and maximum values of each dimension are zero and one, respectively, is typically sufficient. The analysis of the effect of more advanced sampling techniques is left as future work.

Linear scaling is an optional step in AMF that can inserted between the sampling

phase and the forward-mapping phase. When AMF is queried, the points are rescaled to their original values.

6.2.2 Handling Non-Continuous Configuration Spaces

Ordinal (discrete) configuration parameters are handled as a special case in AMF. The sampling program is told whether or not each parameter is ordinal or real-valued. The random selection of data points will abide by this restraint by randomly selecting integers for ordinal parameters, instead of real values

The best way to handle an ordinal parameter in learning the forward mapping depends on the nature of the variable. If the parameter has a wide rage, so that thousands of different values are possible, or if the number has little effect on the system, it may suffice to treat the parameter as a real value. In many cases, the error incurred by making this assumption is negligible. This method has the advantage of providing a common representation across all parameters. Another approach would be to split the configuration space into separate configuration subspaces, with each subspace having a uniform value for the discrete value. This method provides more accurate results at the cost of higher computation requirements. When there are numerous different discrete parameters, however, the number of subspaces grows quickly, making this approach intractable.

6.2.3 Handling Multi-Variate Forward Mappings

Although multiple system-level properties can be measured at once, AMF represents each system-level property as an independent single-property forward-mapping problem. The reformulation of the original definition of the forward mapping is as follows:

$$f_i(\mathbf{x}) \rightarrow y_i$$

where $i = \{0, 1, \ldots, m\}$, where $m = |\mathbf{y}|$. To answer a query for $\hat{\mathbf{y}}$, given $\mathbf{x}$, the sub-mappings are individually queried and collected:

$$\{f_0(\mathbf{x}), f_1(\mathbf{x}), \ldots, f_m(\mathbf{x})\} \rightarrow \hat{\mathbf{y}}$$

This approach assumes that the system-level properties are independent of one another. If this assumption does not hold, the predictions may not be accurate. This problem is outside the scope of the implementation of AMF; the test domains that have been used with AMF, the assumption appears to hold.

6.2.4   Implementation Details

The AMF regression solution to the forward mapping is split into two distinct steps: training and predicting. The training component builds the model and/or pre-processes the data as necessary. The predicting component allows the user and other framework components (e.g., the reverse mapping) to query the regression model. This process is driven by a user-provided regression library that is plugged into the framework.

Training   During training phase of solving the forward-mapping problem, any necessary pre-processing and/or model construction is performed. This process is implemented as a Python function called *train*. Most regression algorithms will store models or metadata in memory for later use. Basic kNN does nothing since the queries use the entire data set. LOESS performs the iterative locally weighted smoothing step to build y' values, which are written to a file. Nonlinear regression learns the optimal parameters for the specified parametric model by using optimization; the parameters for this model are stored. Each of these approaches requires varying amounts of computational time, but needs to be executed only once for a given data set.

Predicting   The prediction phase of solving the forward mapping problem is invoked whenever a query is submitted. This process is implemented as a Python program called *predict*, but is mostly driven by the user-provided regression module. The *predict* function in AMF uses the models generated by *train* to predict values for individual system-level properties.

As in the training phase, the predicting phase is algorithm-dependent, however, the API users interact with is the same. kNN will iterate over each input point to find the nearest neighbors, then average the values. LOESS will interpolate between nearby smoothed training data points. NLR applies the parametric model using the input configuration values. Each of these approaches requires varying amounts of computational time, as with the training step. Since, this process is executed once per query, efficiency is an important factor.

6.3   Using Forward Mapping to Solve the Reverse-Mapping Problem

The forward mapping has two main uses: it is used to predict the behavior of a system, given the configuration; and it is used by AMF to solve the reverse mapping problem. AMF uses the forward mapping to solve the reverse-mapping problem, using one of many of the approaches discussed in Chapter 7. All of these approaches use the forward mapping instead of directly sampling from the ABM for two reasons. First, querying models of the behavior space is faster than interacting with the ABM directly. Second, the regression models smooth the error over the entire space, effectively eliminating natural sampling noise, which can produce more accurate and consistent results.

6.4 Summary

The forward-mapping problem is the problem of developing a mapping that predicts system-level behavior, given the system configuration parameter values. The solution to this problem has a central role in the framework, as it provides the ability for users to predict behavior and is used to solve the reverse-mapping problem.

My solution to the forward-mapping problem is to use regression to learn the correlations between the configuration parameters (independent variables) and the system-level properties (dependent variables), individually. Different regression algorithms, in the form of a Python module library, can be plugged into AMF seamlessly. This allows for a great amount of flexibility in approaches that can be used to sample ABMs. AMF adapts with new technology as new regression techniques are developed since they can simply be plugged in by the user.

Chapter 7

THE REVERSE-MAPPING PROBLEM

The reverse-mapping problem is the problem of defining a function f^{-1} that maps a system-level configuration $\mathbf{y}$ onto a solution space $\hat{\mathbf{S}}$ that represents all possible configurations that would cause the system to exhibit $\mathbf{y}$:

$$f^{-1}(\mathbf{y}) \to \hat{\mathbf{S}}.$$

Every configuration $\hat{\mathbf{x}} \in \hat{\mathbf{S}}$ should satisfy the constraint $f(\hat{\mathbf{x}}) \approx \mathbf{y}$, where f is the forward mapping. That is, $\hat{\mathbf{S}}$ is the set of all the points that would predict $\mathbf{y}$ in the forward mapping.

The major difficulty in solving the reverse-mapping problem is that the mapping is one-to-many because the forward mapping is built with regression (many-to-one). Therefore, querying a reverse mapping returns a solution space, not a singular solution. For this reason, AMF strives to return the *space of configurations* that will exhibit a given system-level property in an ABM, not individual configurations.

This general method of developing a reverse mapping can be contrasted with optimization methods (see Section 9.2). Finding a set of configuration parameters that satisfies a system-level property, by definition, is an optimization problem. However, instead of a single point being returned as in most optimization methods, a reverse mapping returns the space of all points that would satisfy the configuration. This has a number of benefits, such

as being able to visualize and inspect the entire solution space. Analysis of how the solution space changes with respect to the configuration parameters can be performed. Different solutions that produce similar results can be selected from a number of good solutions based on some exterior preference on configurations. That is, although all points in a solution space should be satisfactory, some points may be more desirable for a number of reasons, such as points with lower expected variance.

In this chapter, I give details of how AMF provides two solutions to this problem, in general, then discusses actual implementations of the solutions. Throughout this chapter, I use the NetLogo Fires ABM[1] as an example. The Fires domain is simple and has solution spaces that are easy to visualize. Other domains, such as Wolf Sheep Predation, have too many dimensions to make graphing feasible. The arguments made with the aid of the Fires domain scale to larger dimensions.

7.1   AMF Approach: Simplical Complex Inversion

The first AMF reverse-mapping approach is a novel approach I developed, named *Simplical Complex Inversion* (SCI). A simplical complex is a set of adjacent simplexes (multi-dimensional triangles) that together segregate a space. In abstract terms, SCI builds an invertible approximation of the forward mapping in the form of a simplical complex. This apprach is used because regression is not easily invertible. I have found that inverting even the simplest approaches such as K-nearest neighbor and LOESS are either difficult to implement or computationally expensive (Section 7.3). By approximating a representation of the forward mapping that is invertible, solving the reverse-mapping problem becomes computationally tractable. These direct inversion approaches are generally not preferred over SCI, since they are dependent on the forward mapping approach used and SCI is

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[1]More on the Fires model is discussed in Section 5.1.

applicable to any forward-mapping technique. *SCI is building an invertible approximation of a trained forward mapping.* This is in contrast to building a reverse mapping directly from the training data.

As with the forward-mapping solution, the system-level property $\mathbf{y}$ is split into subspaces to simplify the problem:

$$\mathbf{y} = \{y_0, y_1, \ldots, y_{|\mathbf{y}|}\}.$$

The solution space is split up in a similar manner:

$$\hat{\mathbf{S}} = \{\hat{S}_0, \hat{S}_1, \ldots, \hat{S}_{|\mathbf{S}|}\}.$$

By performing this split, each forward mapping can be inverted independently:

$$f_i^{-1}(y_i) \rightarrow \hat{S}_i.$$

Recombining the individual $\hat{S}_i$ into $\hat{\mathbf{S}}$ is not as simple as recombining individual $\hat{y}_i$ into $\hat{\mathbf{y}}$ in the forward-mapping solution. Since each solution space represents which configurations satisfy a particular system-level requirement, the solution space $\hat{\mathbf{S}}$ is the intersection of all of these spaces:

$$\hat{\mathbf{S}} = \hat{S}_0 \cap \hat{S}_1 \cap \ldots \cap \hat{S}_{|\mathbf{S}|}.$$

All points at the intersection of these spaces should satisfy all system-level properties at once.

Simplical Complex Inversion has three phases. First, regression is used to infer the system-level property values for several "knots"[2] in the configuration space. The locations

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[2]The term "knot" is taken from Multilinear Interpolation(Davies 1997) (section 9.3).

of these knots are used to segregate the configuration space into a number of simplexes. This segregated configuration space is referred to as a *simplical complex* (Munkres 1993). Next, the intersection between each of these simplexes and a plane representing the target system-level property is found. That is, SCI derives the equation of the hyperplane through each simplex that satisfies the target system-level property. A piecewise linear representation the configurations that would satisfy the target system-level property is pieced together from all the intersections. Figure 7.1 illustrates the SCI process; the rest of this subsection dscusses these steps in detail.

Start with the raw data set

Infer knots with the forward mapping

Perform Delaunay Triangulation (ignoring system-level property values)

Each individual simplex spans system-level property space.

Find the intersection between each simplex and the query plane
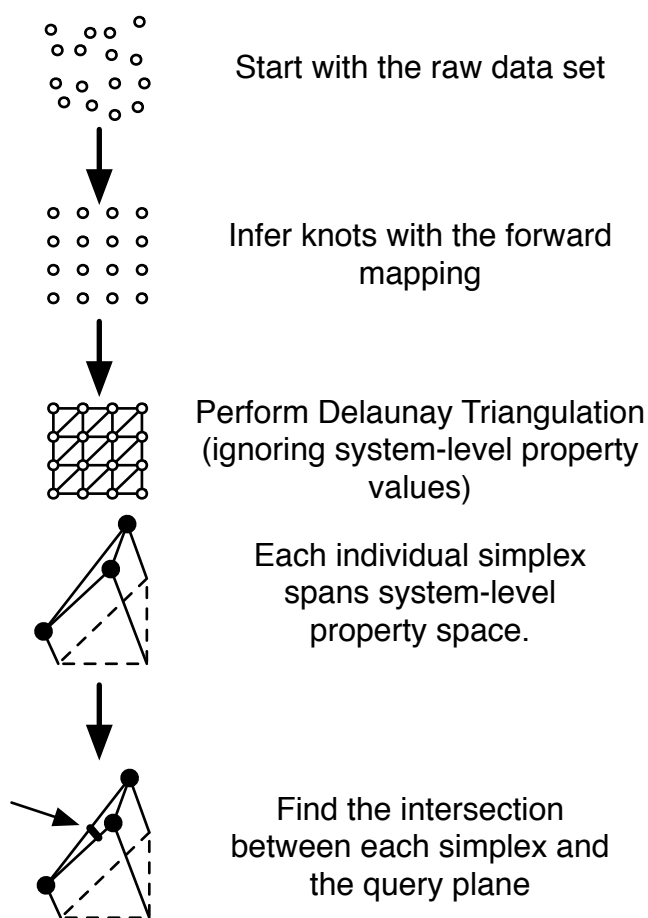
FIG. 7.1. The flow of stages in the Simplical Complex Inversion approach to the reverse-mapping problem in a two-dimensional configuration space.

I claim that SCI is a general approach to the reverse-mapping problem that is applicable in all domains in which the forward-mapping problem is solved accurately. Also, SCI provides more useful information than optimization, since SCI returns the *set* of all configurations. These hyperplanes give a more continuous and complete view of the nature of a specific system-level property value than individual points.

Number of trees burned down in the "Fires" domain
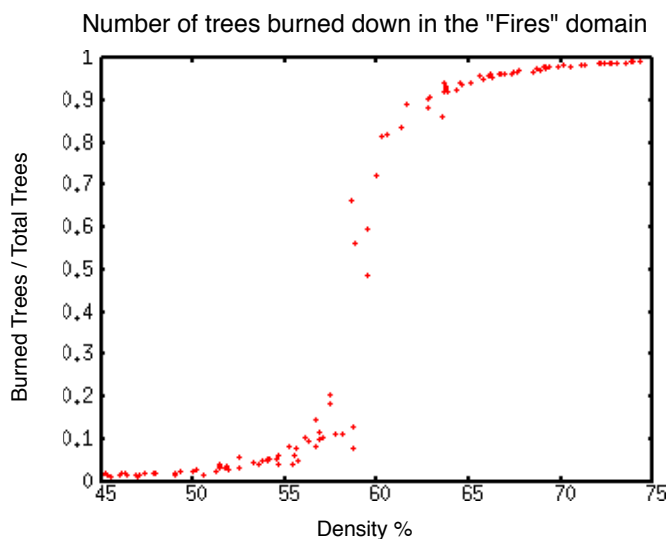
FIG. 7.2. The raw data set, containing 120 points, from the Fires domain.

7.1.1 Segregating the Configuration Space

The reason for using regression as the first step is that the raw data in many ABMs will exhibit variance. For example, raw data from the Fires ABM is shown in Figure 7.2. If this data were to be used with interpolation, the curve for the behavior space would be very erratic. This is a problem for SCI because erratic curves will result in a number of inaccurate intersections. A linear interpolation performed on the raw Fires data to generate a behavior space curve is shown in Figure 7.3. From this figure, the curve appears very erratic and would provide poor results with SCI.
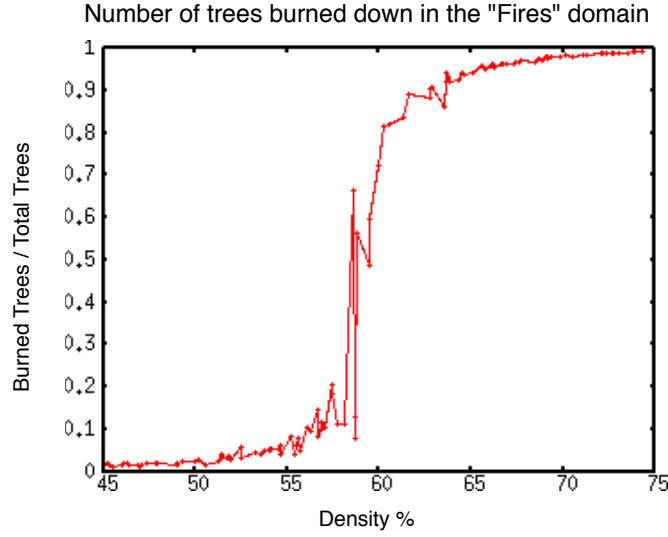
FIG. 7.3. Linear interpolation performed on the raw data set (see Figure 7.2) from the Fires domain.

The behavior space is naturally much smoother when mapped to the regression space. The first step of SCI is to use the forward mapping (i.e., regression) to infer knots in the space, which are evenly distributed across the range of sampled values. The granularity of the knots is specified by the user. These knots cover the space and provide reference points for the interpolation. To generate these points, the forward mapping is queried by passing a complete vector of configuration parameters. An inferred system-level property value is returned. Each data knot in an n-dimensional[3] configuration space is represented by a vector of configuration space parameter values ($\mathbf{x}$) and the system-level property value (y):

$$< x_1, x_2, ..., x_n, y > .$$

The configuration space is then segregated with Delaunay triangulation(Delaunay 1934) into adjacent simplexes (simplical complex). These simplexes have $n + 1$ corners

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[3]n refers to the dimensionality of the configuration space for the rest of this chapter.

(e.g., they are triangles if $n = 2$ and lines if $n = 1$) and spans $(n + 1)$-dimensional space. Note that the behavior space resides in $(n + 1)$-dimensional space, but the simplexes are n-dimensional objects (e.g., a tetrahedron in four-dimensional space if $n = 3$ space or a line segment in two-dimensional space if $n = 1$). This is because the system-level property y is not taken into consideration for the the Delaunay triangulation. The relationships between these objects' dimensionality and different dimensional configuration spaces are outlined in Table 7.1. For example, in the Fires ABM (1-dimensional configuration space), the space is segregated into line segments that reside in two-dimensional space.

Table 7.1. Dimensionality of Objects for Simplex Inversion

Configuration Space Dimensionality	Behavior Space Dimensionality	Simplex	Intersection
1	2	line	point
2	3	triangle	line
3	4	tetrahedron	plane
4	5	pentachoron	3D hyperplane
5	6	5-simplex	4D hyperplane
⋮	⋮	⋮	⋮
n	$n + 1$	n-simplex	$(n - 1)$D hyperplane

If the configuration points were randomly scattered, a standard algorithm for computing the Delaunay triangulation could be used. However, since SCI controls how configuration points are distributed, it can organize the points in such a way that a solution to the Delaunay triangulation can be computed implicitly. In general, SCI will evenly space the sample points as a grid and split each hypercube into two simplexes. The Delaunay triangulation is trivial to compute with points organized in this way. For example, in Figure 7.1, the space is segregated into a number of adjacent triangles that satisfy the requirements for being a Delaunay triangulation. To segregate the space into a Delaunay triangulation from a regular grid, each hypercube is split into two simplexes. The two simplexes are defined

as the simplex defined with all the corners except for the corner closest to the origin, and as the simplex defined with all the corners except for the corner furthest from the origin. For example, with a square, two triangles are formed with two opposite corners as the right angles for their respective triangles.

The equations of the simplexes can be defined in terms of the hyperplane in which they reside. The $n+1$ points define a n-dimensional hyperplane. If a point is within all the facets and lies on the hyperplane, the point is on the simplex. For example, in the Fires ABM, the two points defining a line segment reside on a line that extends infinitely in both directions. Meanwhile, the facets are defined by the points individually. If a behavior space point lies on the line and resides between the two facet points, the point is a plausible configration that would generate the desired system-level behavior. This explanation expands to two-dimensional configuration spaces, which has triangles as simplexes and line as facets. If a point lies on the plane defined by the the points, and is within the boundaries of the line segment facets, the point is realistic.
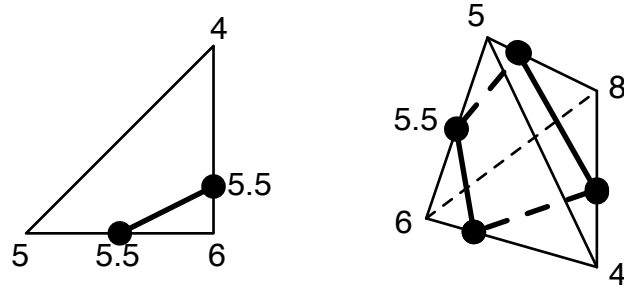
FIG. 7.4. A triangle from a two-dimensional configuration space (left) and a tetrahedron from a three-dimensional configuration space (right) are intersected with the plane $y = 5.5$. The y-values for each corner are given.

7.1.2 Simplex Intersection

Recall that the final goal of this process is to find the equation of the intersection between all the simplexes and a system-level property hyperplane. Therefore, no complicated technique needs to be performed to calculate the actual equation of the simplex or the facets. Edge intersections are used to approximate the intersection through the simplex. The process to find the intersection between the system-level property hyperplane and a simplex is as follows:

1. Pair off each corner with every other corner, in every possible combination. These point pairs define the edges of the simplex.

2. Determine which edges intersect with the hyperplane. An edge intersects with the hyperplane if the target system-level property value is between the y-values for the two points that define the edge. From the intermediate-value theorem, the plane must intersect with this line segment at some point, at least once.

3. Use linear interpolation to determine at which point on the edge line segment the intersection occurs. For example, suppose that the corners have y-values of 2 and 4 and the target system-level property value is 3. The location of the intersection is halfway between the corners.

4. The set of all edge intersection points lie on the hyperplane that intersects the simplex. Use these points to define the intersecting hyperplane.

This approach circumvents the need for modeling the actual simplexes as equations, which can be challenging to implement. Two illustrative examples of this intersection method are shown in Figure 7.4. In the example on the right-hand side in Figure 7.4, the two-dimensional plane intersects the tetrahedron in four places. However, only three of these

points are needed to define the plane because the fourth point is coplanar and thus re-dundant. This illustrates the fact that not every edge has to be checked for intersection, only enough points to define the intersecting hyperplane. Since the intersecting hyperplane is $(n-1)$D, n points are needed. SCI uses the following standard representation for a plane, where $\mathbf{C}$ is a vector of constants and $\mathbf{x}$ is the vector of configuration parameters and system-level property:

$$\mathbf{C} \cdot \mathbf{x} + D = 0$$

$$C_0 x_0 + C_1 x_0 + ... + C_n x_n + C_{n+1} x_{n+1} + D = 0.$$

This approach is very general and will work in most cases; however, when the plane intersects with either a corner point or an edge only, no plane can be defined because not enough non-colinear points can be found. To circumvent this problem, SCI considers the boundaries of the simplex as not part of the simplex. Thus, a point that intersects with only the corner or an edge will not be considered in the final piecewise intersection.

7.1.3   Recombination of Solution Spaces

Once solution spaces have been found for each of the desired system-level properties, they are recombined into one solution space. This final solution space will be a piecewise hyperplane function, consisting of points that exhibit the specified system-level property values. Since the individual reverse mappings are hyperplanes, the recombination is the intersection of all these hyperplanes.

First, SCI verifies if the hyperplanes intersect within the simplex. Two hyperplanes intersect if the points on one hyperplane are separated by the other hyperplane. If the points are separated, then there must be an intersection. An illustration of points being separated by a hyperplane, and not, is shown in Figure 7.5. This intersection check is performed by plugging in values for the edge intersections of one hyperplane into the equation of

On different sides   Both on same side
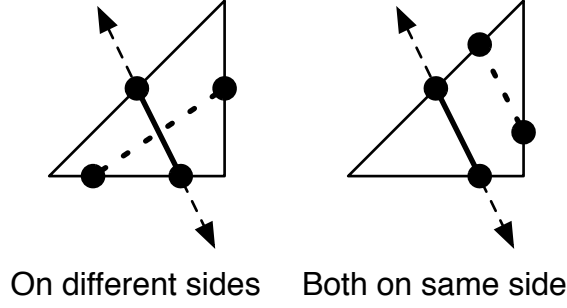
FIG. 7.5. Illustration of two recombination scenarios: intersecting (left) and not intersecting (right).

other hyperplane. Then, the nature of the inequality (greater-than or less-than) for each point specifies which side the edge intersection is on. If one point is on the other side of another point, the planes intersect. This calculation is easy to perform since SCI has the edge intersection points and the equation of the hyperplanes already computed. Also, this process can be repeated for any number of hyperplanes by performing this test for each possible pair of hyperplanes. However, it may be the case that the hyperplanes do not intersect in the same places, even if all of the hyperplanes intersect, pairwise.

To find the intersection, a system of linear equations is set up in matrix form:

$$
\begin{bmatrix}
C_{0,0} & C_{0,1} & ... & C_{0,n+1} & D_0 \\
C_{1,0} & C_{1,1} & ... & C_{1,n+1} & D_1 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
C_{m,0} & C_{m,1} & ... & C_{m,n+1} & D_m
\end{bmatrix}
\begin{bmatrix}
x_0 \\
x_1 \\
\vdots \\
x_{n+1}
\end{bmatrix}
= \mathbf{0}
$$

To solve this system of equations, SCI reduces the coefficient matrix to reduced row echelon form (RREF). What remains is a system of reduced linear equations that are more concise in defining the intersection. From the check performed as the first step, any intersectios returned by the solution of this system of equations is guaranteed to be within the

simplex.

The RREF can reveal that the system is either overspecified or underspecified. A system of equations is overspecified if there is a row in RREF that is all zeros, except for the last column value $D \neq 0$:

$$\begin{bmatrix} 0 & 0 & ... & 0 & D \end{bmatrix}.$$

This row translates to $0 = D$, which is not true. That is, there is no possible configuration of $\mathbf{x}$ that will satisfy this specific equation. Thus, the set of system-level properties the user has provided is not able to be created with this ABM. This is typical if the user has specified too many requirements of the system-level properties. In this case, the user should remove some less important system-level property requirements and allow the system to suggest values for them.

RREF reveals that the system is underspecified if there are any rows with multiple non-zero values in it, other than D. For example, consider the row pulled from a matrix in RREF:

$$\begin{bmatrix} 0 & 1 & 2 & 0 & 5 \end{bmatrix}.$$

This row translates to $x_1 + 2x_2 = 5$. Therefore, x_1 and x_2 are free variables, but are still constrained by this equation. An infinite number of solutions can satisfy the system-level properties in this case. This is not a problem like being overspecified, since there are a number of possible solutions available to the user.

7.1.4 Granularity

SCI can be configured by adjusting the granularity of the knots. SCI approximates an invertible continuous representation of the forward mapping. Therefore, as the granularity of SCI increases, it models the forward mapping more accurately. Thus, the granularity should be as high as computationally acceptable.

Granularity can be adjusted dynamically on a query-by-query basis. Individual simplexes may be separated into several subsimplexes. These new simplexes are composed of the original simplex's corners, in addition to new corners. The new corners have their system-level property value inferred from the forward mapping. Once these new simplexes have been formed, nothing special has to be performed to accommodate them in the general SCI algorithm. In addition, even if the granularity has been increased for a specific query, the finer grained simplexes can remain to increase the accuracy of future queries.

Dynamic adjustment of the granularity process can be performed automatically to increase the accuracy of simplexes that contain significant amounts of variability between the system-level property values at the corners. Increasing the granularity will reduce the variance, since points closer to one another will have increasingly similar values.

The effect of the granularity on accuracy is dependent on the nature of the forward-mapping regression method used. If the forward-mapping produces overfit or otherwise inaccurate predictions, the reverse-mapping produces will be inaccurate as well. This difficulty should be dealt with in the forward-mapping solving step, not the reverse-mapping solving step. This is because the purpose of SCI is to model the forward-mapping, not the domain.

An empirical analysis of the relationship between granularity and accuracy is provided in Chapter 8. The accuracy is measured as the approximate total difference between the continuous forward-mapping function and the continuous simplical complex. In addition, suggestions made from SCI are validated against an actual system run of the target ABM. The error between the desired system-level property values and the actual system-level property values are measured. This measurement is redundant, since the error between the actual run and the reverse-mapping solution should be the sum of the forward mapping error and the reverse mapping error (in respect to the forward mapping).

7.1.5   Example: Fires ABM

Figure 7.6 illustrates the progression of SCI from step to step when used for the Fires ABM. First, the forward-mapping problem is solved, with any regression method. Then, the knots are formed in evenly spaced intervals: in this case intervals of 1% tree density (see top right image in Figure 7.6). The simplexes in the case of the Fires ABM are line segments, since the configuration space is one-dimensional. Therefore, linear interpolation between the points produces the simplexes (see bottom left image in Figure 7.6). Each segment is also the only edge of the simplex.
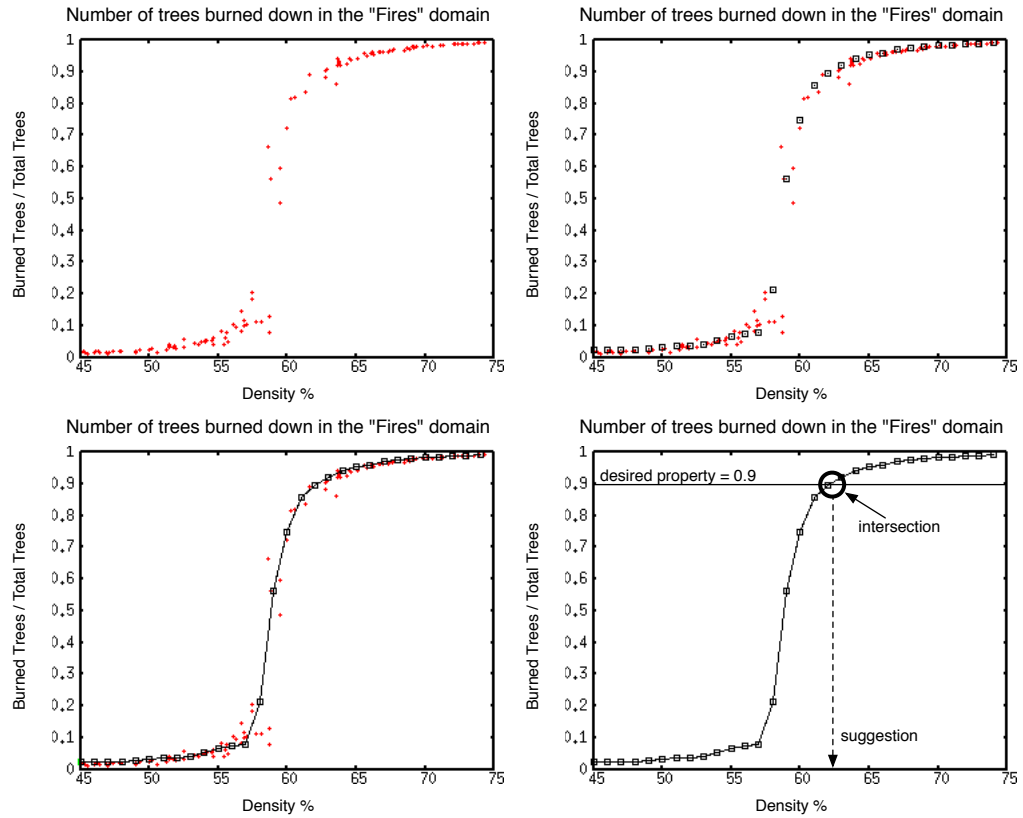
FIG. 7.6. The progression of SCI in the Fires ABM from raw data set (top left), to intersection (bottom right).

Next, SCI finds the intersection between the behavior space and a desired system-

level property behavior $b = Burned\ Trees/Total\ Trees = 0.9$ (see bottom right image in Figure 7.6). This is done by checking each simplex to see if 0.9 is within the range of the minimum value and maximum value for b in each simplex. The only segment that intersects the 0.9 plane is the one between 63% and 64%. The intersection between this segment and the line is calculated, which in this case is approximately at $Density = 63.1\%$.

Therefore, setting $Density = 63.1\%$ will be expected to yield 90% of the trees burned down. In higher-dimensional domains, the number of points that will satisfy the system-level property will be infinite instead of just one point, since they lie on a continuous hyperplane.

7.1.6 Special Cases

In this section, I discuss two special cases that can simplify the SCI process significantly. Users of AMF can see significant improvements in computation time if either of these cases can be identified as a property of a domain.

Classification System-level properties that are binary (positive and negative) in nature (i.e., the forward-mapping is classification, not regression) can be treated differently. SCI handles binary-valued system-level properties by labeling each simplex as either:

- positive – corners are all positive instances,

- negative – corners are all negative instances, or

- inconclusive – corners are a mixture of both positive and negative instances.

Then, once a query is submitted with binary values as part of the requirement, SCI removes all simplexes that do not match that binary value. For example, if a query contains a positive binary value, all negative and inconclusive simplexes are removed from the search.

Inconclusive simplexes are removed since there are probably a number of simplexes which will satisfy the system-level property constraint. This is possible because these simplexes will not be part of the solution, even if other system-level properties could be satisfied by configurations within these simplexes. This shortcut can significantly reduce computation time if a majority of the space is removed.

Inconclusive simplexes are situated on the boundary of positive and negative instances in the space. Therefore, the granularity of the inconclusive simplexes can be increased by separating them (Subsection 7.1.4) in order to reduce the amount of space occupied by inconclusive simplexes.

One-to-One Mapping With some properties, the forward mapping may define a one-to-one mapping. If this is the case, then regression can be used for the reverse mapping by training on the system-level property to infer values for the configuration parameters. The regression will return the single configuration that satisfies the system-level property, since it is one-to-one. Therefore, if a user is working with a one-to-one mapping, this should be the only property being analyzed. Only one point is returned, so adding additional constraints will typically over specify the system of equations and not return anything.

The percentage of trees burned down in the Fires ABM is an example of a one-to-one relationship, since the percentage of trees burned down increases monotonically with the density of the trees.

7.2 Alternative Approach I: Optimization

In related work, researchers typically treat the problem of finding a configuration that will satisfy some system-level constraint as an optimization problem.[4] In this type of approach, an optimization meta-heuristic such as simulated annealing or genetic algorithms can be used to incrementally adjust the system configuration until the system-level properties match the final goal. These approaches use a concept of fitness that measures the actual outcome with the expected outcome. ABMs that exhibit closer outcomes are weighted higher so that the algorithm gradually converges on a solution.

The main reason that this approach is a poor choice for the reverse-mapping problem is that sampling the ABM on every iteration can be very slow. To calculate the fitness of a particular configuration, the ABM must be executed and measured. Running the Wolf Sheep Predation model takes at least one second per run. Every generation of a genetic algorithm could have to execute an ABM several hundred times, which case, each generation could take several minutes to compute.

A hybrid approach is possible that significantly reduces the online running time of optimization. Instead of directly sampling the ABM, the optimization technique can use the forward mapping to infer the outcome of a configuration instead of executing it. This approach also has the benefit that the regression smooths the predictions, which in many cases will give more consistent results than querying an ABM directly. This approach is effectively searching through the regression space created by the forward mapping, which is an approximation of the true behavior space.

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[4]Section 9.2 summarizes related work in which researchers treat inverting the forward mapping as optimization.

7.3   Alternative Approach II: Functional Inversion

Some regression approaches can be directly inverted. This has the benefit that no approximation, such as SCI, has to be performed, however, a functional inversion is algorithm-dependent, meaning a new method must be implemented for each regression.

I will provide functional inversions of kNN and NLR, as examples. kNN is conceptually and computationally difficult to invert. The "forward mapping" of kNN is: What is the average of the values for the k nearest point to configuration vector $\mathbf{c}$? The inverse of this statement is: What space covered by k neighboring points would produce the average p? One way to compute this, would be to generate a structure similar to a Voronoi diagram that segregates the space into sections. Every point within a section has the same k-nearest neighbors, which is iterated over to find averages that are close enough. This search can be computationally intensive as the number of sections can be large with large high values for k. Also, since this space is discontinuous, finding a desired average may be impossible. With SCI, continuous transitions are inserted between the discontinuous spaces, allowing intersections to be inferred, even if no average exists.

Nonlinear regression, on the other hand, is rather simple to invert with algebra, with certain parametric models. Basically, inverting NLR reduces to satisfying the following equation:

$$f(\mathbf{x}, \beta) - y = 0,$$

where β are the learned model parameters and y is the desired system-level property value. This equation can be solved with a number of numerical root finding methods. Inverting nonlinear regression, in particular, is useful because it provides an elegant solution in the form of mathematical equations, instead of the piecewise ones provided by SCI.

7.4   Using Reverse Mappings

The main purpose of generating a reverse mapping is to gain understanding of the space of configurations that generate a particular system-level behavior. The relationships between configuration parameters can be inferred by analyzing these spaces. For example, when one configuration parameter value is reduced and the other is increased a specific amount, the resulting system-level behavior may be the same. The equations returned by SCI provide this mathematical representation in a piecewise way. This deeper understanding of how a system-level property can be produced is more faster and potentially more valuable than having a researcher manually study a domain to gain understanding of how the configurations affect system-level behavior.

The reverse mapping can be used to suggest a configuration when a user wishes to see a particular behavior exhibited in the ABM. For example, suppose the user of AMF wants to determine what an execution of a Fire ABM that burns down 80% of the trees looks like. SCI can suggest what density of trees should be used. Typically, the user would have to go through an iterative process of guessing a possible configuration, then executing the ABM to determine if the configuration generated the behavior or not. This is effectively manual hill climbing, and can be unintuitive, difficult and tedious.

To suggest a configuration with AMF, the user queries the reverse mapping with the desired system-level property values. SCI returns the space of configurations that would satisfy this query. Any point in this space will be satisfactory; however the user must select one. Whether this point is selected arbitrarily or not is up to the user. To select an arbitrary point, a random simplex is chosen. Then, a set of values that will satisfy the system of equations associated with that simplex are derived. Free variables have their values randomly selected, within the range of the simplex. The fixed variables are fixed, so their values are already given. Together, these points provide the user with a suitable point

in the solution space to configure the target ABM.

Certain points in the solution space can be considered better than others, even if they should produce similar output. Typically, areas of the space that have minimal variance are safer choices for configuration suggestions, since the expected error is less. As an aside, the action of removing high variance areas of the space is possible by adding a binary valued system-level property that separates the space into "high variance" and "low variance" spaces, given a specified threshold. This approach has the benefit that the selection of configurations with low variance is performed inside the framework, instead of by the user.

7.5 Summary

The reverse-mapping problem is the problem of finding a one-to-many mapping that maps system-level property values to the set of ABM configurations that would exhibit that behavior. AMF uses one of two algorithms I devised, named SCI and QT, that build an *invertible* approximation of the forward mapping. This approximated mapping can be inverted and thus return the inverse of the forward mapping. Results detailing the computational time required offline, the computational time required per query, and the accuracy of the reverse mappings developed by AMF are discussed in Chapter 8.

Chapter 8

RESULTS

In this chapter, I discuss experiments that test the accuracy and computational efficiency of AMF. These experiments also serve as examples of AMF being applied to a variety of ABMs. In the next section, the different evaluation criteria are outlined. Each of these metrics will be applied to a number of domains using a number of different techniques for the forward mapping. The four domains used for the sake of experimentation were outlined in Chapter 5. Each of these domains have unique properties that provide unique challenges to show the versatility of AMF. The different regression methods for the forward mapping are outlined in Section 8.2. Finally, in Section 8.3, the statistical results are discussed.

8.1 Evaluation

Evaluating AMF is important because it shows that the framework is a practical and useful tool for studying ABMs. Evaluation is split into two processes: evaluating the forward mapping solution and evaluating the reverse mapping solution. Accuracy of these mappings in modeling the behavior space of the target ABM is paramount in importance. If the forward and reverse mappings are not accurate, there would be no reason to use this framework for investigating behaviors of ABMs. Computation time is also an important

factor in evaluating AMF. Interactions with the user need to be quick in order to make using AMF more convenient than manually inspecting the target ABM. The response time of when a user interacts with AMF is the *online* time and is far more important than the *offline* time, the one-time computation requirement to learn the forward or reverse mapping.

8.1.1 Forward Mapping

Accuracy   Accuracy is the measurement of how closely the forward mapping represents the true behavior space of a target ABM. To measure this, the difference (error) ε between the predictions for a system level property $\hat{y}$ that the forward mapping produces and the actual value y for a sampled point: $\varepsilon = |\hat{y} - y|$. This measurement is performed many times for a single domain to produce the median error and the the upper and lower quartiles of the errors.

The errors are gathered by performing cross validation. Two subsets of data points are randomly pulled from the master set of samples to create a training set and a validation set. The forward mapping is built by using the training set, and then checked with the validation set.

The error is calculated for varying size data sets to show the relationship between error and data set size.

Offline Computation Time   Offline computation time is the average amount of system time the forward mapping uses to train a model. This is measured as the amount of time the pre-processing takes, given a training set. The size of the training set is varied to determine how forward mapping training time is correlated to training set size. Each forward mapping method is compared to the others.

Online Computation Time   Online computation time is the average amount of time AMF takes to return the results of a user-submitted query. This is measured by performing a large number of queries and calculating the average run time. The size of the training set can affect the amount of time a query will take with some algorithms. In these cases, the size of the training set is varied to determine how query time correlates to training set size.

8.1.2   Reverse Mapping

Accuracy vs. Forward Mapping   Accuracy of the reverse mapping is measured in two ways. The first is how accurately the reverse mapping models the forward mapping. Recall that AMF solves the reverse mapping by building an invertible approximation of the forward mapping. This metric determines if this approach is doing what is expected to do. The effect that granularity has on this accuracy is also measured by learning the same mapping with increasingly higher granularity.
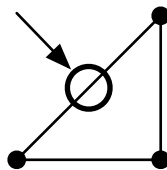
FIG. 8.1. The most erroneous spot in a right-angled simplex.

The error is presented as an "average worst-case scenario". The area of the reverse mapping space that is be the most erroneous is typically be the one furthest from the knots (corners of the simplex). An illustration of this point is presented in Figure 8.1. The point is halfway between all corners, except for the corner at the right angle. This point is the most erroneous if the forward mapping is monotonically changing from one side of the simplex to the other (i.e., there are no local maxima or minima within the space). Note that the reverse mapping will be identical to the forward mapping at the knots, since the forward

mapping was used to infer their values.

Calculating the approximate upper bound on error, within a simplex, involves interpolating the system-level property value at the most erroneous point. This is done by average the system-level property values of all corners not at the right angle. Also, the location of the most erroneous point is queried for prediction through the forward mapping. The difference between the interpolated value on the simplex and the actual predicted value using the forward mapping constitutes the error. This metric is applied for every simplex and then averaged. Thus, the metric measures the average error over all the worst-case scenarios for each simplex. Also, the distribution of these errors is recorded to convey how consistent the reverse mapping is.

Accuracy vs. Agent-Based Model Run   The main goal of the reverse mapping is to be able to suggest configurations that would generate a specified behavior. This approach is different from the previous metric because it measures the difference between the reverse mapping and the true behavior space.

Closest point is an
edge intersection

Closest point is
within the simplex
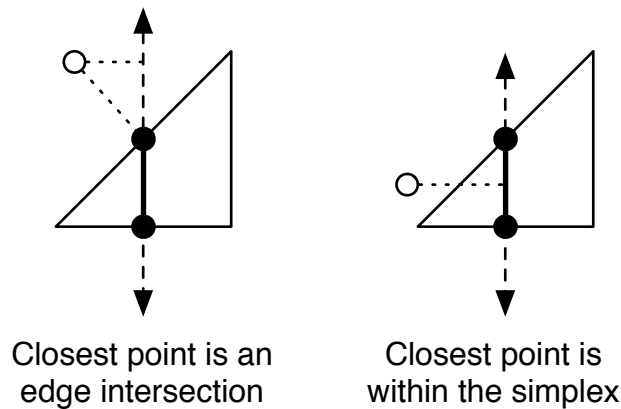
FIG. 8.2. Two cases for the closest point to a simplex intersection.

Error is measured by generating a random configuration point and sampling it from the agent-based model. Then, the system-level property that was measured is passed to

AMF to generate a reverse-mapping solution. The error is the distance from the original configuration and the reverse-mapping solution space. This value is calculated by adhering to the following procedure, per simplex:

1. Determine the distance from the original point to the intersecting hyperplane.

2. If the shortest line from the hyperplane to the point intersects the hyperplane *within* the simplex, then the distance from the hyperplane is the distance from the intersection to the point.

3. Otherwise, the closest point is one of the edge intersections.

The two different cases (closest to an edge (left) and closest to the hyperplane (right)) are illustrated in Figure 8.2. The minimum of all of these closest simplex points is taken as the distance from the actual system-level property value to the piecewise curve generated by the reverse mapping.

Several random configurations are sampled in this way. The average and standard deviation of these errors are calculated to convey the accuracy of the reverse mapping, as well as the consistency of the reverse mapping.

Offline and Online Computation Time Offline computation time and online computation time is measured the same way for the reverse mapping as the forward mapping. The amount of time AMF takes to prepare the reverse mapping is the offline computation time, and the amount of time required to produce a reverse mapping solution is the online computation time.

8.2   Forward Mapping Methods

For the experiments in this chapter, the three algorithms described in Chapter 3 are used for the forward mapping. In the following outline, I indicate specific configuration

parameters or implementation details of importance.

- k-nearest neighbor (KNN)

  - Custom implementation with Python.

  - 10-fold validation is used to determine the best k out of a set of possible k values.

- robust locally weighted regression and smoothing scatterplots (LOESS)

  - Custom implementation with Python.

  - A good window is selected by myself for each domain. Changing this configuration parameter per sample size does not affect accuracy, as it does with kNN.

  - Performs one smoothing operation. I found that increasing the number of smoothing operations past one provided limited improvement in accuracy and occasionally worsening accuracy. Finding an optimal smoothing with cross validation, per training set, would be computationally expensive.

- nonlinear regression (NLR)

  - Implemented in Python and uses the SciPy[1] package to optimize the parametric model with least-squares.

8.3   Experiments

First, I will discuss results from the Fires domain together, which provides an extended example that explains the methodology and results for each of the seven experiments. The

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[1]SciPy is a freely available Python module that has a number of useful computational tools. The SciPy website is: http://www.scipy.org/

rest of the experiments for the other domains are grouped together by experiment, so that the effectiveness of the different components of AMF are evaluated independently.

8.3.1 Fires Domain Experiments

The NetLogo Fires domain is an excellent example for showing how AMF works, as the domain is relatively simple and easy to visualize. Plots of the behavior space for this domain are shown in Figure 7.6.
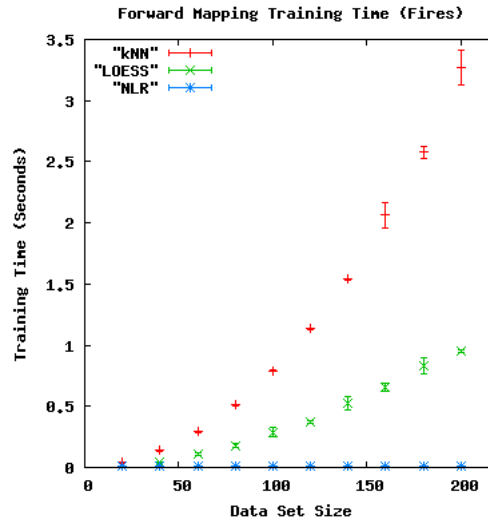
FIG. 8.3. The average length of time required by the forward mapping for the Fires domain to train. The error bars show the 95% confidence interval for the mean.

Forward Mapping Training Time   Different training data set sizes, ranging from 20 to 200 (with a step of 20), were used to measure the amount of computation time the forward mapping requires to train a model. Each of the three regressions were retrained twenty times per training data set size. The results are plotted in Figure 8.3. This plot shows that kNN grows faster than the other two approaches with increasing data set sizes. This is because the 10-fold validation for picking k requires a significant amount of time.

Meanwhile, LOESS grows at a linear rate. The training time for NLR is insignificant in comparison to the other approaches. Least-squares optimization is a mature subject area, and SciPy uses some of the most advanced methods to make the optimization quick.

Even the slowest of these regressions, kNN with 200 training instances, runs in only 3.25 seconds, which is acceptable for a one-time process.

The error bars show that there is little variability in training time, meaning that the approaches are consistent in the amount of time they take.
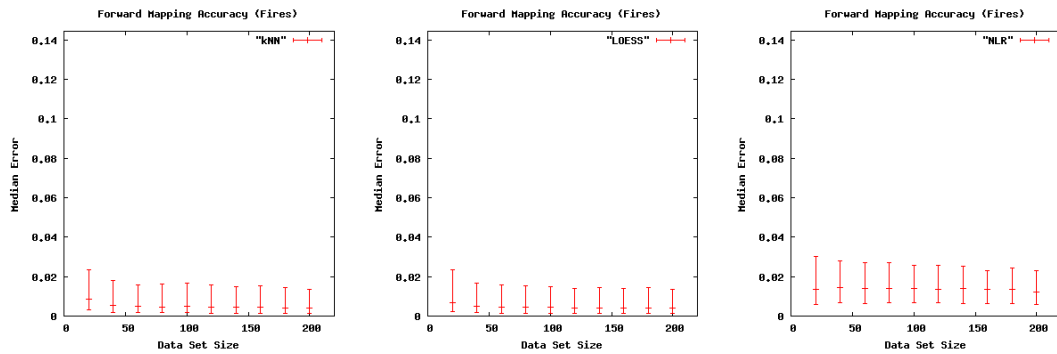
FIG. 8.4. The median error (in ratio of trees burned down) for three different forward mapping regression methods. The error bars show the upper and lower quartile of the errors, over all trials.

Forward Mapping Accuracy   Different training data set sizes, ranging from 20 to 200 (with a step of 20), were used to train a model. Fifteen different training data sets were produced per data set size. For each of these trained models, 2500 points from a validation set were used to evaluate the accuracy of the forward mapping, in respect to values sampled directly from ABMs. The configuration of each validation instance was passed into the forward mapping to retrieve a predicted value. This predicted value was then compared to the sampled value from the validation instance to produce an error value.

The accuracy of the forward mapping is very high, for all three approaches: all three

approaches predict the amount of trees burned down within an accuracy of 1%. The median error, along with the upper quartile and lower quartile are plotted in Figure 8.4.

This is impressive considering to the amount of variability from sample to sample of the Fires domain. Both KNN and LOESS perform better with more data points, however with a sample size greather than 80, the accuracy does not appear affected very much. Overall, KNN had a lower median error than LOESS, but not by a statistically significant amount. NLR performed worse than the other two approaches and experienced more variance in its errors. Interestingly, the accuracy of NLR only slightly improved from a data sample size of 20 to a data sample size of 200. Since NLR is a parametric approach, the optimal model for a small number of points will be very similar to the optimal model for a large number of points from the same distribution. Meanwhile, locally weighted non-parametric approaches have the ability to fit sections of the behavior space more closely as more points are provided. This trade off is demonstrated in the accuracy results.

FIG. 8.5. The average number of seconds required to query the Fires forward mapping. The error bars show the 95% confidence interval for the mean.

Forward Mapping Query Time   Measurements of the query time were performed at the same time as the accuracy measurements. The elapsed time was measured for every prediction call to the forward mappings.

Queries to the forward mappings for the three approaches are fast, as illustrated in Figure 8.5. The longest time for a query to execute was .0045 seconds for LOESS using a data set of size 200. This amount of time is instantaneous to a human user and thus satisfies the requirement that the forward mapping is fast for the user. As expected, data set size has no effect on the computation time of NLR because the model equation is always the same number of parameters. Also, as expected, LOESS and kNN query time grows linearly with the size of the data set. For every new point added, an additional point must be checked to see if it is local to the passed in configuration, or not.
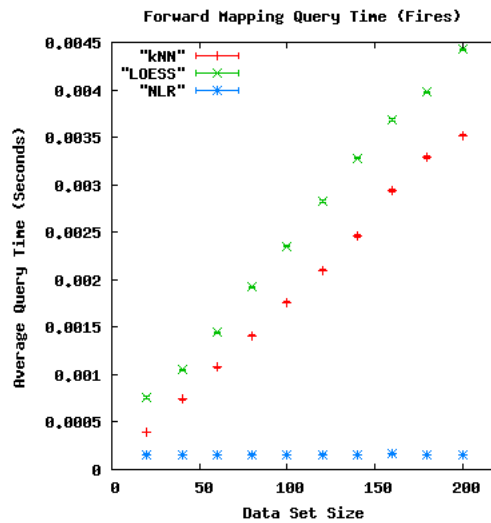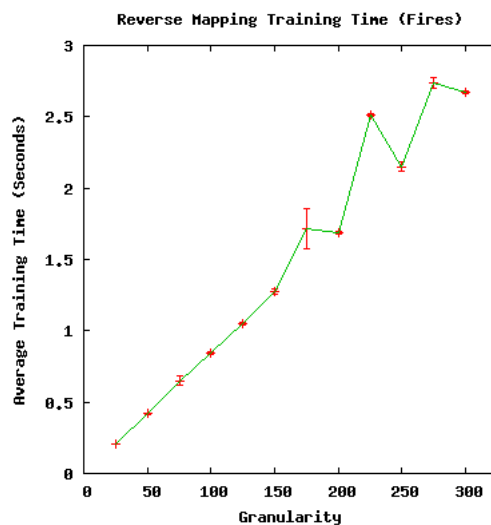

FIG. 8.6. The average number of seconds required to train the Fires reverse mapping. The error bars show the 95% confidence interval for the mean.

Reverse Mapping Training Time   The most accurate forward mapping trained in the previous forward mapping experiments was used for the reverse mapping experiments.

In this case, I used kNN with a training set of 200. Training time was measured for reverse mappings training on granularities of 25 to 300 (step 25). A granularity of N means the configuration space was split into N simplexes, per dimension. The test was repeated fifteen times per granularity.

The training time increased linearly with an increase in granularity. With a granularity of three hundred, the training time was under three seconds. With a granularity of twenty-five, the training time was just under a quarter of a second.
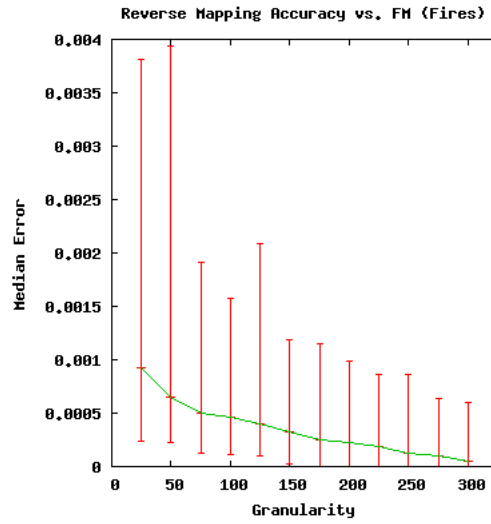
FIG. 8.7. The median distance from the suggested tree density (0-100) to the one predicted by the forward mapping. The error bars show the upper and lower quartile of errors measured.

Reverse Mapping Accuracy   The reverse mapping accuracy is measured in two ways. First, I measured the median error of the reverse mapping in respect to the predicted values of the forward mapping. This metric demonstrates the accuracy of fifteen different reverse mappings per granularity, as an approximation of the forward mapping. This metric is measured by taking each simplex in the reverse mapping and selecting the furthest point

from the corners. Each of these points are then passed to the forward mapping to provide a prediction, which is then compared to the interpolated value within the simplex. The difference between these two denote the error of the values within the simplex, in respect to the forward mapping it is approximating.

Figure 8.7 shows the effect of granularity on median error. The error steadily decreases with higher granularity, eventually approaching 100% for about half of the queries. Also, the error is extremely low in all cases, never exceeding half a percent of trees burned down. The reverse mappings trained with high granularities were often accurate within a tenth of a percent of trees burned down.
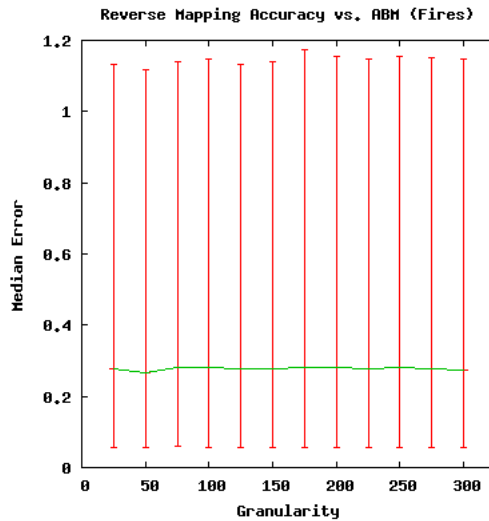
FIG. 8.8. The median distance from the suggested tree density (0-100) to the actual tree density. The error bars show the upper and lower quartile of errors measured.

The second way the accuracy of the reverse mapping is measured is how distant the piecewise configuration curve returned by the reverse mapping is from the actual configuration. Recall that the reverse mapping returns a set of intersections (however, in the case of Fires typically only one, since the mapping is one-to-one). This metric intends to measure the distance from a configuration suggested by the reverse mapping, and the actual

configuration from the validation set. Each of the 2500 instances from the validation set were used for each of the reverse mappings that were trained.

The results in Figure 8.8 show that the median error remains fairly constant, regardless of granularity. The reason for this is that the error incurred by the approximation of the forward mapping is insignificant in comparison to the error of kNN. Since the same kNN forward mapping was used for all granularities, the error incurred by the reverse mapping is not noticeable or statistically significant.
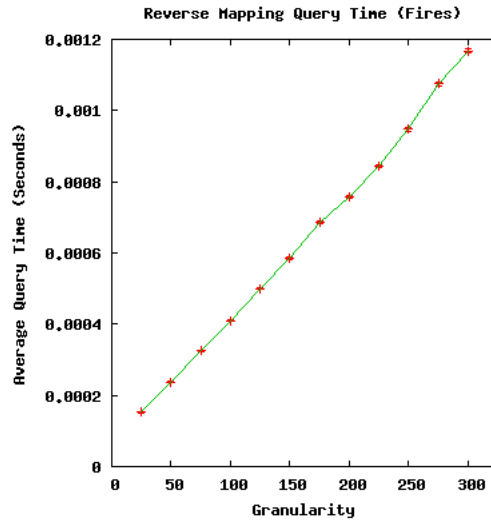
FIG. 8.9. The average number of seconds required to queury the Fires reverse mapping. The error bars show the 95% confidence interval for the mean.

Reverse Mapping Query Time   The reverse mapping query time was measured along with the accuracies of the reverse mapping, in respect to the validation set.

Overall, the average reverse mapping query computation time is almost instantaneous, taking about 0.0012 seconds with a granularity of 300, as seen in Figure 8.9. The average query time increased linearly with the granularity because each additional simplex must be checked for intersections.

8.3.2 Forward Mapping

Accuracy   The accuracy of the forward mapping was measured in the three remaining domains (Flocking, AIDS and Wolf Sheep Predation). In all domains, both k-nearest neighbor and LOESS outperformed the baseline of predicting the mean value over all system-level property values. Also, all experiments demonstrate that, in general, accuracy increases as data set size increases. However, the decrease in error from increasing data set size is not a linear relationship, as the benefits of larger datasets lessens as the size increases. In general, kNN performed better than LOESS. Non-linear regression has been omitted from these experiments for the reason that it is difficult to determine a suitable base-model and initial guess for a multi-dimensional space.
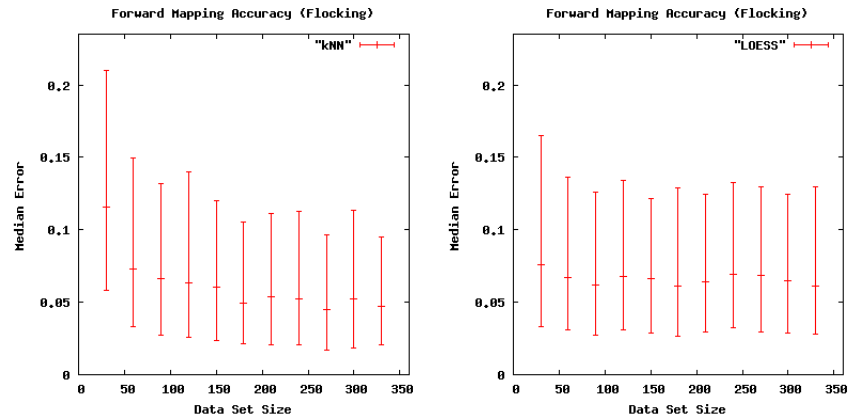
FIG. 8.10. The median error for the standard deviation of heading (on a zero-to-one scale) in the Flocking domain for two different forward mapping regression methods. The error bars show the upper and lower quartile of the errors, over all trials.

Both LOESS and kNN were tested for training a forward mapping to predict the standard deviation of heading in the Flocking ABM. A forward mapping was trained fifteen times for each data set of the same size, each being queried one thousand times. Plots showing the relationship between data set size and median error are shown in Figure 8.10.

KNN outperformed LOESS, but not significantly, eventually approaching a median error of .05 with a training set size of 325. LOESS approached an error of .06 with the same training set size. These error values are linearly scaled such that the maximum standard deviation witnessed is exactly 1.0 and the minimum standard deviation witnessed is exactly 0.0. The baseline is not shown in these graphs because it is not within the y-range of the plot: on average, predicting the mean value had an error of .306, over all 4000 data set instances.
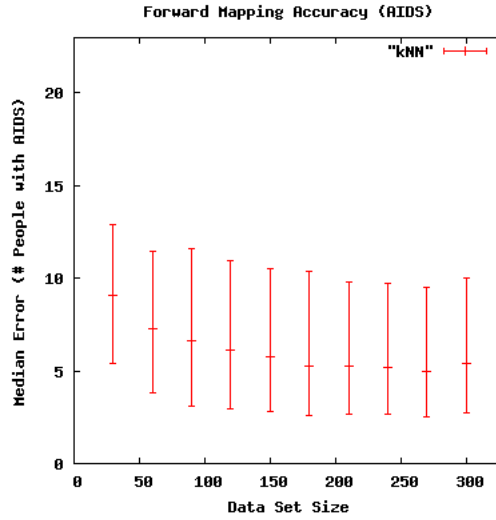
FIG. 8.11. The median error showing the difference in people (out of 350) between the original curve and the curve predicted by the forward mapping, on average, over all time steps. The error bars show the upper and lower quartile of the errors, over all trials.

Four forward mappings were trained to predict four parameters of a generalized logistic function that models the number of people with HIV, in respect to time. The model used was:

$$y = p_0 + \frac{p_1 - p_0}{1 + e^{-p_2(t - p_3)}},$$

where $\mathbf{p}$ is the vector of parameters $p_0, p_1, p_2,$ and p_3 and t is the time step. As the data set size increases from 25 to 300, the median error drops from nine people to just over five, as

seen in Figure 8.11. This error is measured by taking the average difference between the predicted curve and the actual curve from the validation set. To calculate this, the value for each time step, for both functions is calculated. The deviations are averaged, which yields the median error plotted in Figure 8.11.

Note that the AIDS domain technically does not adhere to one of the major assumptions used in AMF: in order to split the forward-mapping problem into several subproblems, the system-level property values must be independent of one another. This is not the case since all the parameters are part of the same model function. However, I found that in this particular case, the forward mapping predicted the values of the HIV population adequately.
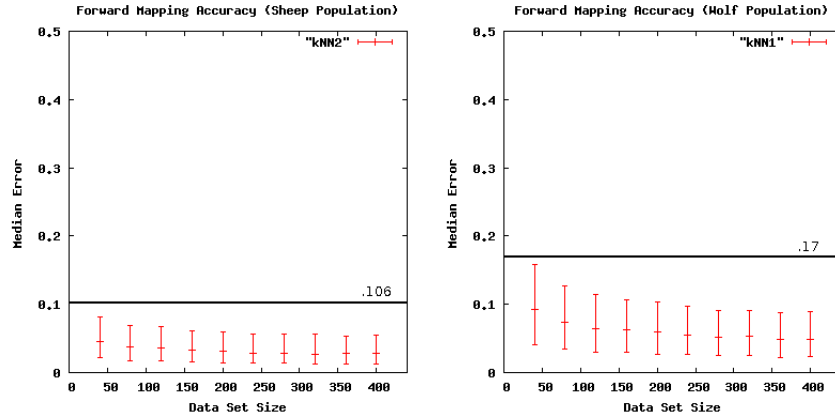
FIG. 8.12. The median error in the average number of sheep (left) and the average number of wolves (right), scaled from zero to one. The error bars show the upper and lower quartile of the errors, over all trials. Predicting the mean population value yields an error of .106 and .17 for sheep and wolf populations, respectively.

The next round of experiments tested the effectiveness of the forward mapping approach in predicting four properties of the Wolf Sheep Predation domain: the average sheep population, the average wolf population, the sheep population variance, and wolf extinction. A forward mapping was trained eight times for each data set of the same size, each

being queried two hundred times. The forward mappings outperformed simply predicting the mean value in all four cases, with sufficient training sets.

The median errors for the wolf population and the sheep population are shown in Figure 8.12. As the training set size approached 400, the error for the sheep population forward mapping approached 2% of the range of values in the data set, which is five times more accurate than predicting the mean. The forward mapping for the wolf population was more difficult to learn, which is evident from the baseline of .17 being significantly higher than the baseline for the sheep population prediction. The median error for the wolf population forward mapping approaches 4% of the range of values in the data set, which is 4.25 times more accurate than predicting the mean.
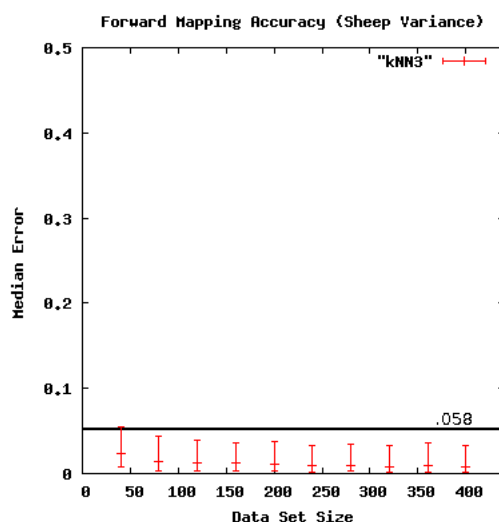
FIG. 8.13. The median error of the variance in the number (scaled from zero to one) of sheep. The error bars show the upper and lower quartile of the errors, over all trials.

Forward mappings were used to predict the variance in sheep populations. Populations with higher variance fluctuated more than ones with lower variance. The median error for predicting the variance, based on data set size is shown in Figure 8.13, along with a baseline of .058. With a training set size of 400, the learned forward mapping outperformed the

baseline five-fold.
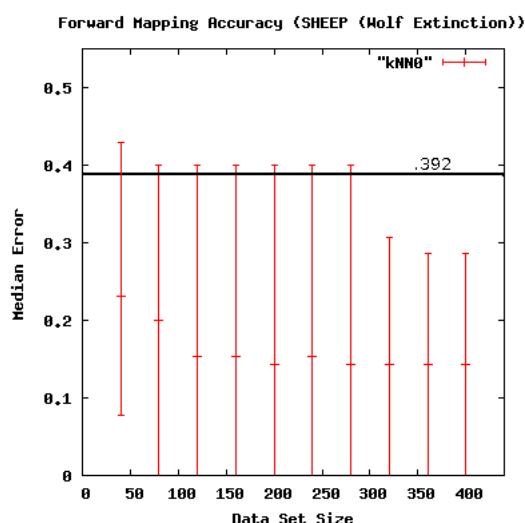
FIG. 8.14. The error in prediction of the wolf population going extinct or not. The error
bars show the upper and lower quartile of the errors, over all trials.

Next, forward mappings were used to predict whether or not the wolf population
would go extinct. This property is different from the others, since it is a binary prop-
erty: either the wolves go extinct or they do not. The forward mapping solution predicts
the probability that the wolves go extinct, so the errors shown in Figure 8.14 do not quite
have the same meaning as the other plots. The data in the training set is either labeled as
wolves having gone extinct or not. Therefore, a prediction of .9 would yield an error of
.1 if the wolves went extinct, and an error of .9 if they did not. From the plot in Figure
8.14, we can see that a forward mapping can be used to predict if the wolves will go extinct
correctly the vast majority of the time (at least 75%). Also, with a data set size of 400, the
forward mapping is more than twice as accurate in comparison to the baseline.

In conclusion, the AMF approach of solving the forward-mapping problem is suffi-
ciently accurate in predicting system-level behavior in these domains.

FIG. 8.15. The average number of seconds required to train the Flocking (left) and AIDS (right) forward mappings. The error bars show the 95% confidence interval for the mean.

Offline Computation Time Offline computation time refers to the required amount of time to train a forward mapping. Recall that kNN determines the best k using 10-fold cross validation and LOESS performs the initialization and smoothing step. To measure the average training, several forward mappings for all three domains were trained for varying data set sizes. Figure 8.15 shows the training time for the Flocking domain and the AIDS domain. Even with training sets as large as 350, the forward mappings were able to be trained in less than 2.5 seconds for the Flocking domain and 8 seconds for the AIDS domain. Figure 8.16 shows the training time for the Wolf Sheep Predation domain, which yields a similarly shaped curve. The difference in training time between domains, even if the data set size is the same, is directly resultant of the number of system-level properties because each is learned individually. Note that if kNN had k preselected, it would require no training time.

Online Computation Time Online computation time is the average time required to query the forward mapping. Since the forward mapping intends to replace the need for manual experimentation with ABMs, the forward mapping query should be significantly

FIG. 8.16. The average number of seconds required to train the Wolf Sheep Predation forward mapping. The error bars show the 95% confidence interval for the mean.

Table 8.1. Average Time for Individual Runs of ABMs

ABM	Average Time Per Run (seconds)
Fires	0.17
Flocking	8.20
AIDS	4.61
Wolf Sheep Predation	6.51

faster than actually running the ABM. The average number of seconds required to query each of the ABMs in these experiments are listed in Table 8.1. As shown in Figure 8.17 and Figure 8.18, the average query time is far below that of actually running the ABM. For example, about two thousand Flocking forward mapping queries can be performed per Flocking ABM run. Both LOESS and kNN have a linear rate of growth, which is as expected, because as more points are added to the training set, the more points that must be iterated over. Naturally, problems with more system-level properties will require more time.
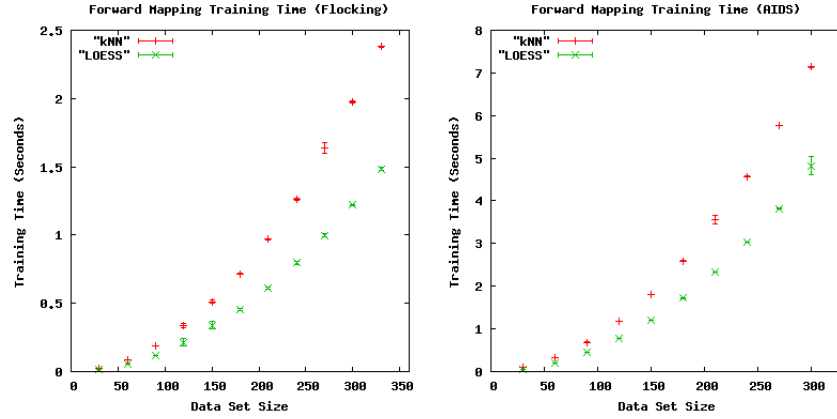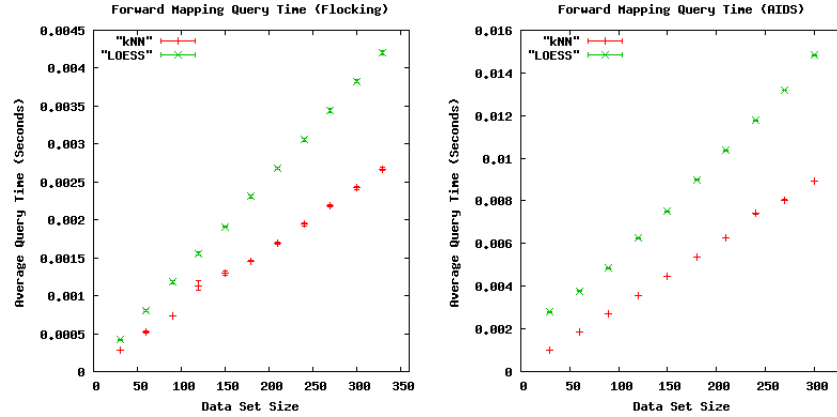
FIG. 8.17. The average number of seconds required to query the Flocking (left) and AIDS (right) forward mappings. The error bars show the 95% confidence interval for the mean.

8.3.3 Reverse Mapping

Accuracy vs. Forward Mapping   The accuracy of the reverse mapping is measured as how well it approximates the forward mapping. To measure this, for each simplex in the reverse mapping, the center point of the simplex has its system-level property values predicted with the forward mapping, and with the average the values at the corners. The values at the knots have no error, since they were generated with the forward mapping. Therefore, the points furthest away from these corners are most likely to have the greatest error.

Results for the accuracy of the flocking domain are shown in Figure 8.19. The median error of the reverse mapping with a granularity of 40 is about .007, which pales in comparison to the .05 error (see Figure 8.10) between the forward mapping and the actual ABM. Therefore, the error incurred by the reverse mapping is relatively insignificant, especially when sometimes the error can cancel out the forward mapping error (i.e., the error from the reverse mapping and forward mapping is not additive).

Similar conclusions can be made about the accuracy of the reverse mapping for the
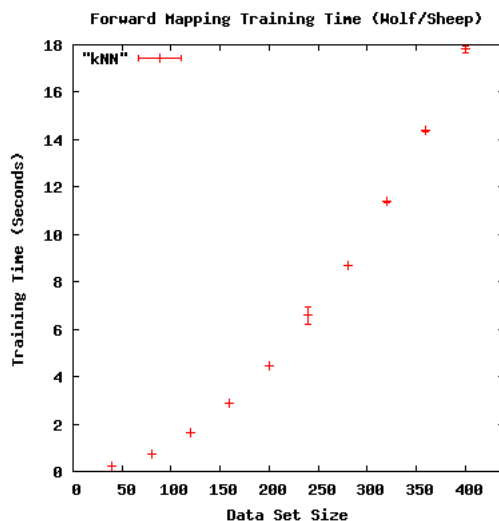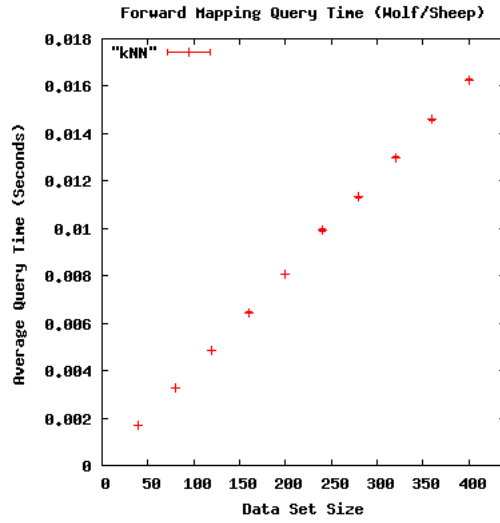
FIG. 8.18. The average number of seconds required to query the Wolf Sheep Predation forward mappings. The error bars show the 95% confidence interval for the mean.

AIDS domain, which are plotted in Figure 8.20. The median error for this domain with a granularity of 50 is below one person. That is, in the most erroneous place in each simplex, the reverse mapping will predict the forward mapping's prediction within one person. This error is about six times less than the error incurred by the forward mapping, for this domain.

Offline Computation Time   The process of training the reverse mapping involves querying the forward mapping to generate the knots and then building the simplical complex from these knots. Figure 8.21 shows the training time, based on granularity for the Flocking and AIDS domains. At 40 granularity, the reverse mappings required approximately 9 seconds and 225 seconds to train for the AIDS domain and the Flocking domain, respectively.

For both the AIDS and Flocking domains, the required amount of time to train is acceptable, since it is computed offline. However, there is a very large difference for the same granularity, given just one dimension difference in the configuration space (AIDS
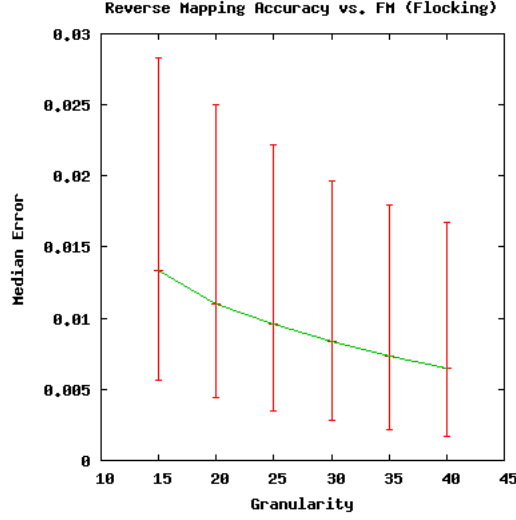
FIG. 8.19. The median difference in the forward mapping and the reverse mapping in predictions for the Flocking domain. The error bars show the upper and lower quartile of errors measured.

has two configuration parameters, while Flocking has three). Unfortunately, the training time and memory is exponential in respect to the dimensionality. Since each dimension is split granularity g times, there are a total of $2g^d$ simplexes, where d is the dimensionality of the configuration space. The coefficient of "2" comes from the fact that each grid location is split into two simplexes. Therefore, the memory required and the computation time required grow quickly with more dimensions. The results from the Wolf Sheep Predation (with a configuration space dimensionality of five) are omitted because a granularity low enough to allow the experiments to run in a reasonable amount of time yielded poor accuracy.

Possible general methods for avoiding this computational problem are left as future work, which include optimization using the forward mapping and scaling granularity. The simplest fix is to sample less configuration parameters at once and to learn individual reverse mappings for subsets of the configuration space. Much information and qualitative
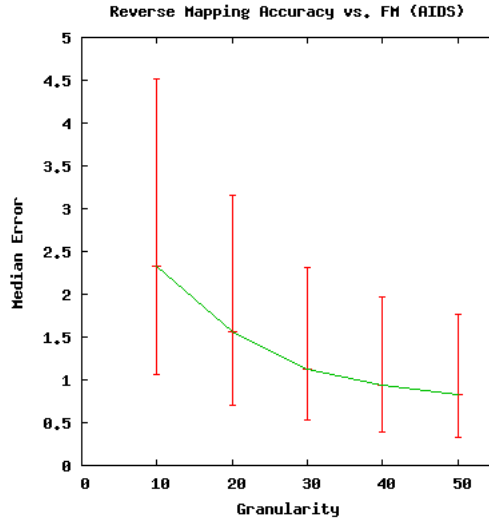
FIG. 8.20. The median difference in the forward mapping and the reverse mapping in predictions for the AIDS domain. The error bars show the upper and lower quartile of errors measured.

information can still be gathered from these smaller mappings.

Online Computation Time   Querying a reverse mapping requires the submapping for each system-level property to be searched for intersections. Each simplex must be checked for intersections, so the running time of the query is based directly on the number of simplexes. Since the number of simplexes grow at $O(g^d)$, the query is polynomial time, in respect to granularity. This relationship is reflected in the results shown in Figure 8.22. Similar to the training time, the query time for Flocking and AIDS are significantly different due to the additional configuration dimension in the Flocking domain. In both these domains, queries were generally less than half a second, which is acceptable performance.
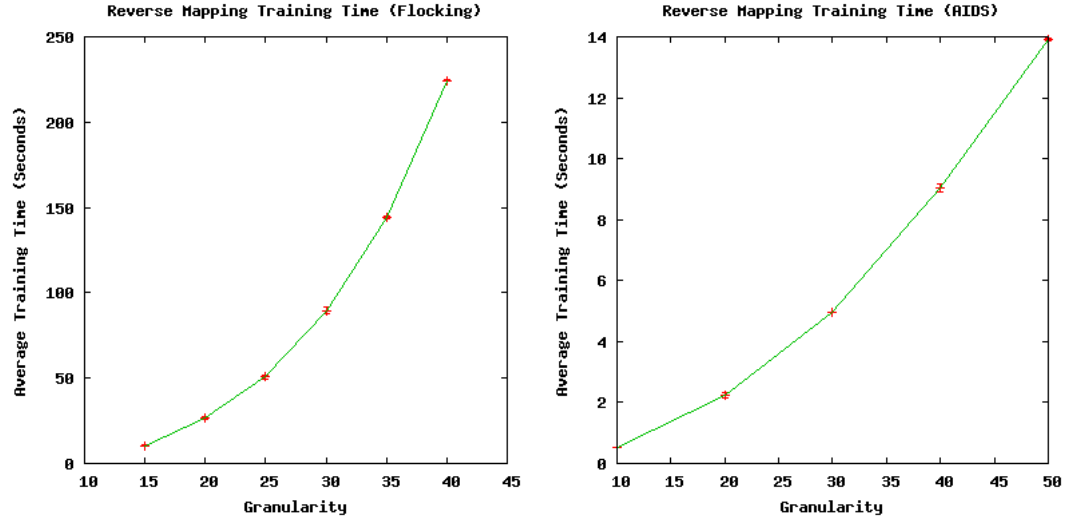
FIG. 8.21. The average number of seconds required to train the Flocking (left) and AIDS (right) reverse mappings. The error bars show the 95% confidence interval for the mean.

8.4 Summary and Conclusions

In summary, the forward mapping performed exceptionally well in comparison to the baselines provided. The forward mapping is an accurate and quick tool for predicting real-valued system-level properties, as well as predicting the probability of a threshold effect (such as wolf extinction). AMF was able to provide a general solution to this problem, proven by applying the same approaches to all four domains.

The reverse mapping solutions generated by AMF model the forward mapping accurately. However, the computational and space complexity grow quickly with dimensionality, which make this approach intractable for highly-dimensional domains. For the one-, two-, and three-dimensional configuration spaces presented in the results, granularities of forty produced accurate results within a reasonable about of time.
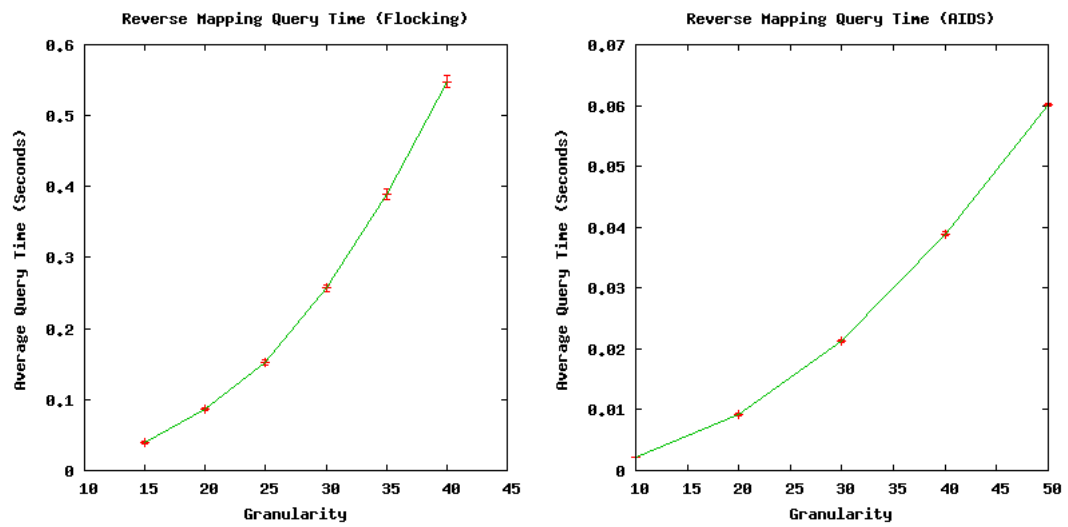
FIG. 8.22. The average number of seconds required to query the Flocking (left) and AIDS (right) reverse mappings. The error bars show the 95% confidence interval for the mean.

RELATED WORK

A number of different research projects have had similar motivation to the different compartments of AMF, but no other projects have attempted to build a comprehensive behavior space mapping system. This chapter compares related work to AMF, and notes ways in which AMF has improved the state of the art in ABM behavior space modeling. In Section 9.1, several projects in which researchers experimented with different configurations of ABMs are summarized. Then, in Section 9.2, different attempts at inverting the forward mapping are discussed. Finally, Section 9.3 gives an overview of Multilinear Interpolation, which was the inspiration for the simplical complex method for solving the reverse-mapping problem.

9.1 Experimentation in ABMs

There is a large body of experimental work using a simulation of a particular domain. Researchers are typically either attempting to optimize a particular behavior or to match some desired system-level behavior. Most of these approaches use exhaustive experimentation: a large number of configurations are sampled, and then the authors draw qualitative conclusions based on their findings. These projects provide motivation for developing a forward mapping, because much of the analysis in this particular field is done manually,

which is not necessary with a system such as AMF. Also, more informed qualitative assessments could be made by researchers with the additional information provided by the functional mappings generated by AMF.

9.1.1 A Platform for the Analysis of Artificial Self-organized Systems

Perhaps the system most similar to AMF in motivation is an ABM experimental platform developed by Bourjot and Chevrier (2004). Their platform has the goal of being an automated and domain-independent system for determining under which conditions an expected system-level behavior occurs and for validating a system against true training data. The system provides sampling functionality for the user that finds the mean behavior of several agent-level configurations. Once the data has been collected, plots can be generated that visualize how agent-level parameters affect the system-level properties. The authors suggest that these data sets and plots can be a useful tool for making qualitative conclusions about the domain and the effect of changing agent-level parameters. AMF offers a superset of the features provided by the Bourjot and Chevrier platform. The AMF sampling system automatically samples the behavior space, which can then be passed into a plotting program to generate visualizations. In addition, AMF takes the approach of experimenting with different configurations of an ABM by learning the forward mapping to develop a functional representation of the space.

9.1.2 Experimentation in Realistic Biological Models

ABMs have been used to study behaviors in multi-agent models of biological systems such as ant colonies, locust swarms, and fish schools. Researchers are typically interested in understanding how the agent-level policies that are followed by the individuals produce interesting system-level behavior.

Buhl et al. (2006) studied a model of marching locusts in order to discover the critical density at which locusts start swarming, as opposed to acting independently. At low population densities, locusts ignore their counterparts and graze for food as individuals. Once a certain critical density of locusts is reached, they begin to swarm and collectively destroy crops. Since experimenting with thousands of locusts is infeasible, the researchers utilized an agent-based model that simulates the behaviors of individual locusts. The simulation exhibited the system-level threshold effect of swarming and not swarming, and the researchers were able to determine the value of the critical density through experimentation. The authors note a few system-level properties that describe the swarming behavior, and presented plots that show the relationship between the agent-level configuration and these system-level properties. This work is an example of manual experimentation, in contrast to AMF's automated approach. Also, AMF would enable the researchers to specify a realistic critical density (i.e., one that has been observed in nature) and have the framework determine the set of configurations that would exhibit this critical density. This tool would greatly enhance the ability for researchers to adjust their models to match true domain data.

Couzin et al. (2003) used an agent-based model of a population of ants to study how multiple "traffic lanes" form from many ants leaving and entering a nest simultaneously. The authors found that at low ant densities, agents come and go randomly, without much concern for colliding with other ants. At higher densities, lanes that optimize traffic flow form dynamically. In the experiments, the authors adjusted the avoidance turning rate (i.e., the angular velocity at which an ant is willing to turn to avoid another ant) and the perception angle ahead of the ant (i.e., the ant's field of view) in order to determine the effect of these parameters on the system-level lane formation behavior. The values for the agent-level configurations were plotted against the traffic flow of the ants to demonstrate the correlation. Turning rates and fields of view that were too low resulted in slow traffic flow, probably because the ants did not avoid one another enough, resulting in a number of

collisions or ants waiting for other ants to pass. Turning rates and fields of view that were too high resulted in slow traffic flow, as well, probably because the ants overcompensated to avoid other ants. By plotting the data, researchers were able to determine the configuration of turning rate and field of view that would yield the optimal traffic flow. In addition, the authors experimented with having different turning rates for incoming and outgoing agents different. They found that if the outgoing agents had a higher turning rate than the incoming agents, the ants formed a three-lane system: incoming ants in the center and outgoing ants split, approaching the nest on the sides. Intuitively, this property results because the incoming ants are less willing to avoid the outgoing ants, forcing the outgoing ants to the outside. This lane formation is observed in army ants in the real world. The authors found that increasing the difference between turning radii in outgoing and incoming ants generally increased the efficiency of traffic flow. Most of the analysis that was done in this work was assisted by the plot visualizations of the behavior spaces. In more complex domains with more dimensions, plotting may not be possible. In cases such as these, models of the behavior space generated by AMF can be useful for making qualitative conclusions based on the data.

Parrish et al. (2002) developed a generalized model of fish schooling that aggregates concepts from several schooling models. In these models, a population of fish form into several subgroups or "schools." The authors emperically measured the effects of agent-level parameters on a number of school-level and population-level statistics, such as group size, number of groups, stragglers, collisions, and polarization. Several different types of repulsion/attraction curves (the definition of how fish are attracted or repulsed by one another, based on distance) with different shapes and magnitudes were tested. The authors draw a number of qualitative conclusions about the effects of agent-level parameters on the system-level properties. They found that environmental factors such as drag and randomness had little effect on fish schooling behavior, in comparison to the social forces, such as

avoidance. With a convex attraction-repulsion curve, fish stayed closed together and had more collisions; however, the polarization (i.e., agreement on direction) was unaffected. Changing the magnitude of neighbor scaling to have social forces be higher weighted based on distance made fish schools smaller and faster and decreased collisions.

9.1.3 Experimentation in Particle Swarm Optimization

Particle swarm optimization (PSO) is a swarm intelligence technique for finding a solution to optimization problems in a multi-dimensional, continuous search space (Kennedy & Eberhart 1995). PSO uses a multitude of agents that "swarm" around good solutions, hoping to find better solutions. Agents in PSO are in predetermined neighborhoods in which all members of the same neighborhood share the neighborhood's highest fitness found. Each agent keeps track of its personal highest fitness found, its neighborhood's highest fitness found and the global highest fitness found. Then, an agent moves towards each of these maximum fitnesses with predetermined weights, specified by a parameter provided by the user. Additional parameters specify the number of agents and how much momentum agents have (defined as how much of the agent's velocity vector in the previous time step is carried into the next time step).

PSO originally provided no guidelines for determining appropriate settings for the following parameters: the number of neighborhoods, the size of the neighborhoods, the constants in the force equation (personal best factor, neighborhood best factor, global best factor, momentum), the maximum speed of the agents, the initial spread of the agents, and the initial velocity. One of the first attempts at developing a methodology for selecting parameter values was an empirical study of different configurations for particle swarm optimization (Shi & Eberhart 1998). The authors performed experiments to measure how the inertia weight (the momentum of a particle) and the maximum speed affect the performance of PSO. The intuition behind this experiment is that if particles are too fast (i.e., have high

inertia and high maximum speed), they will overshoot optimums, missing them entirely, while particles that are too slow (i.e., have low inertia and low maximum speed) will take a long time to reach optimal solutions. A number of different configurations were used and the results are presented as a table. There is no way to determine if these parameter values will transfer to target domains other than the experimental one.

A more general approach was attempted in a study by Van den Bergh and Engelbrecht (2006), which provides a more theoretical perspective to particle swarm optimization than the previously discussed empirical research. The focus of this work is to determine which configuration parameters will cause particles to converge on a good solution, as well as to predict the nature of the particle trajectories over time. However, although this paper provides theoretical results for PSO, the authors explicitly state that the paper is not an approach to determining optimal parameters and points readers to empirical studies. AMF can analyze systems such as PSO to find configurations that perform as expected, which takes the empirical studies one step further than just sampling data points by aggregating information from them.

9.1.4   Models of Multi-Agent Systems

The research summarized so far in this chapter used exhaustive experimentation to draw conclusions about the behavior space of a system. In the two projects described in this section, meta-models (i.e., models about the model) of the system are defined and used to draw conclusions about the system.

Physicomimetics is a physics-based system for controlling multi-robot teams that was developed by Spears et al. (2004). In this system, agents are considered objects that behave according to classic physics equations, such as $\vec{F} = m\vec{a}$. Agents can perform a number of self-organizing tasks with these rules, such as forming hexagonal lattices and square formations. The major benefit of using a physics-based control policy is that the system

behavior can be analyzed using the equations, instead of having to experiment with the system. System designers of this framework can avoid costly trial-and-error of the controllers by deriving theoretical laws from the controlling functions. This benefit is similar in motivation to AMF: provide a way to interact with a multi-agent system with models, rather than experimentation. Analysis of the system grounded in mathematics is useful and precise, but will not extend to domains other than the one it was designed for. Spears et al. specifically designed physicomimetics with the meta-model in mind, which is not possible for all ABMs; by contrast, the approach taken by AMF is applicable to many more domains. This work was the main inspiration for using nonlinear regression as one of the forward-mapping methods. Physicomimetics demonstrates that there are many benefits to having a concise mathematical model for a system: the ability to predict behavior by using equations and being able to prove concepts about the domain by interacting only with the model. However, the main difference between this approach and AMF is that the physics models in physicomimetics were designed by human intuition, while the models built by AMF are constructed using machine learning techniques and therefore domain-independent.

"Macroscopic models of swarm robot systems" (Lerman & Galstyan 2002; Lerman, Martinoli, & Galstyan 2005) are similar in motivation to AMF, but models the system in a more specific way (as finite state machines), and is therefore limited to systems in which agents can be modeled as FSAs. My approach is more general, since it builds its models from system-level parameters of any type of ABM. Lerman et al. (2002, 2005) propose a novel approach to modeling a multi-agent system comprised of finite state machine agents. Since each robot is a finite state machine, this approach models agents as stochastic Markov processes (i.e., processes in which future state depends only on present state). Next, several functions $N_x(t)$ are developed that predict the average number of agents in state x at time t, which have a number of uses:

- Describe how the system will behave over time and whether or not it will eventually

converge.

- Summarize how much cumulative time has been spent in each state, which is useful for determining more abstract measurements of the system-level behavior. For example, the authors demonstrate the efficiency of a system based on how much cumulative time the agents spent avoiding one another, as opposed to foraging.

- The length of time a task will take can be predicted. For example, if it is known that a total amount of m minutes must be spent foraging to complete the task, one can determine the time step at which the integral of N is m.

The authors used two domains: collaborative stick pulling and collaborative foraging. They found that with more agents, the robots spend more time avoiding one another and less time collecting. From this, the authors were able to determine how the efficiency of each robot is affected by group size, through experimentation. The N functions representat the system-level properties and are analogous in many ways to the AMF forward mapping. However the approaches are fundamentally different because the functions are based on time t, not on the configuration of the system. Also, requiring the agent behaviors to be describable as a Markov decision process limits the number of domains to which this research could be applied. AMF is agnostic to the representation of the agent, which makes AMF more general.

9.2   Inversion of Forward Mappings

The reverse-mapping problem has been tackled before by "inverting" the forward mapping. The idea is not new, but AMF's approach of returning a functional approximation of the reverse space is novel. All of these the previous approaches return a single solution, rather than a space, and many of these approaches are online. This greatly reduces the usefulness of these approaches in making conclusions about the domain.

Learning the reverse mapping is typically an ill-posed problem because if the forward mapping is many-to-one, then the reverse mapping is a one-to-many relationship. The major problem with directly learning this type of mapping is called the "convexity problem" (Jordan & Rumelhart 1992): if the set of all possible solutions does not form a convex space, then the average of the inputs may land outside this space, and will therefore yield a poor result. Many techniques, such as KNN and LOESS, depend on the average to generate accurate results. For example, approaches that simply directly learn the reverse mapping as a supervised learning problem, such as work by Widrow and Stearns (1985), will not work in mappings that are not one-to-one.

Much work has been done in inverting multilayer neural networks and most of these approaches use some sort of optimization technique. The goal is to determine which inputs to the neural network will generate a specified output. These approaches do not return a mapping, which AMF does, but instead find a single solution that satisfies the desired system-level property. Also, these techniques are tailored specifically for use with neural networks and are therefore not algorithm-independent. Two such approaches are:

- Linden and Kindermann, "Inversion of multilayer nets" (1989) – The authors use gradient descent to minimize $\sum (Y_i - f(X_i))^2$ by adjusting X_i. That is, they incrementally adjust X_i such that the difference between the desired output Y_i and the actual output $f(X_i)$ is minimized.

- Lu, "Inverting feedforward neural networks using linear and nonlinear programming" (1990) – The author formulates the inverse problem as a linear programming problem and then uses a modified simplex method approach to solve it. This approach has the benefit of being able to specify exterior constraints with linear programming. Also, various points can be derived by setting different constraint functions, which allows the user to control the location of the output point. With a gra-

dient ascent approach, the region of the output point is unknown and unpredictable, which can be a problem in some situations.

Some more general approaches have been attempted for inverting the forward mapping in an algorithm-independent manner. Lee and Kil (1989), present an iterative approach that can approximate any continuous function. The algorithm incrementally approaches a better solution, and escapes local minima to continue searching for more solutions. However, one requirement for running this approach is that the Jacobian must be calculated (or approximated), which makes this approach difficult to apply to certain functions, such as piecewise or discontinuous ones. The authors suggest that their approach would work well with neural networks, since the Jacobian for a neural network is easy to compute. As with the other approaches, this one returns one solution.

Stonedahl and Wilensky (2010) use evolutionary search to look for non-convergence in the NetLogo Flocking and V-Formation Flocking (similar to flocking except that agents form into "V" formations) domains. Their approach uses genetic algorithms to search the configuration space for a particular system-level property of interest, or to optimize a particular behavior. In particular, genetic algorithms are used to find the configuration that converges to a single heading as fast as possible. This approach requires a quantitative measure of the system-level properties, similar to defining system-level properties in AMF. An interesting addition to this approach is that it plots the results as a set of box-plots that show the ranges and distribution of configurations that generate desirable behaviors, which provides additional insight into the nature of the system-level behavior than optimization methods that return an individual point. However, the correlations between the configuration parameters are mostly ignored in these plots. That is, the ranges are shown, but how a single point in one parameter solution space maps to another one is not clear. This approach is similar to ours in how it strives to build a representation of the reverse mapping; however, since the correlations between the system-level properties are not explicitely

visualized, this mapping cannot be queried—it can only be used as an aid for qualitative analytics. By contrast, AMF's reverse mapping can be queried to return a multi-dimensional solution space that describes all satisfiable configurations.

9.3 Multilinear Interpolation

Multilinear interpolation is a dynamic approach that uses multi-dimensional interpolation between "knots" to generate a smooth surface across a space of any dimensionality (Davies 1997). Knots are sampled data points, scattered across the behavior space in a regular fashion such that the knots, when connected, form hypercubes. When a point $\mathbf{x}$ is queried, multidimensional interpolation is performed using the corners of the hypercube to infer the value of $\hat{y}$. A major downside to standard multilinear interpolation is that the sampling needs to be systematic and evenly spaced. To remedy this situation, another regression algorithm can be used to compile a set of evenly spaced points. AMF's simplical complex inversion uses this approach so that it can use randomly sampled data. These evenly spaced inferred points are then passed to a traditional multilinear interpolation approach.

Multilinear interpolation serves as an inspiration for my SCI approach. They are practically identical, except that SCI segregates the space into simplexes, instead of hypercubes (see Chapter 7). This modification was necessary because intersections can be found at the edges of simplexes and connected with straight line segments. Slices through a gradient in a hypercube that represent a particular value are not linear. Therefore, the representation is more complicated and makes working with them more difficult. SCI is therefore less smooth because of the linearity of the pieces, but easier to work with.

Chapter 10

CONCLUSIONS AND FUTURE WORK

In the course of this dissertation, I have outlined the inner-workings of The ABM Meta-modeling Framework. The requirements and strategies for defining system-level properties were enumerated in Chapter 4. The approach AMF takes in solving the forward-mapping problem with regression was explained in Chapter 6 and proven accurate and efficient in Chapter 8. Formulating the problem of prediction system-level properties of an ABM as a regression problem fit naturally. The approach AMF takes in solving the reverse-mapping problem with the novel simplical compelx approach was explained in Chapter 7 and proven accurate and efficient in most cases in Chapter 8. Inverting an approximation of the forward mapping proved to be an accurate and general way to build a reverse mapping to solve the reverse-mapping problem.

The main goal of the ABM Meta-modeling Framework was to bridge the intuition gap between agent-level configuration parameters and system-level property values. The forward mapping can be used by researchers to perform experimentation, but much faster than interacting with the ABM directly. Whether the researcher is currently using an optimization approach or manually inspecting the system, using the forward mapping is more convenient and faster than interacting with the ABM directly. Only a small amount of error is incurred by using AMF, which is greatly outweighed by the benefits. The reverse

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mapping can be used as a replacement for optimization and to provide the space of configurations that will satisfy a system-level property. This is useful for finding a number of configurations that will generate desired behavior in an ABM. Also, researchers can use the reverse mapping as an aide to making qualitative conclusions about the nature of the system-level properties.

In Chapter 2, the following constraints were placed upon the implementation of AMF:

- Domain independent: The design of AMF should minimize the amount of configuration that is needed for each new domain;

- Algorithm independent: any regression algorithm should be able to be applied with AMF;

- Accurate: AMF should generate accurate predictions and control suggestions; and

- Fast for the user: interactions with the models generated by AMF should require minimal computational time.

AMF achieved these goals.

Over the four domains that AMF was applied to, none required special modifications to the implementation of the framework to function correctly. The same interfaces were used for each domain, and can be used for future domains. The reverse-mapping solution simplical complex inversion is algorithm independent, as shown by the fact that the core framework did not have to be modified in order to accomodate k-nearest neighbor, LOESS, or non-linear regression. Future regression algorithms may be used for the forward mapping and the reverse mapping would require no changes. Therefore, AMF is domain and algorithm independent.

The results in Chapter 8 show that the implementation of AMF produces accurate results across all domains that we tested. In most cases, AMF was fast for the user. From the

results, forward mapping queries are thousands of times faster than actually querying the ABM. This is incredibly important for researchers who wish to experiment with ABMs, but do not wish to spend upwards of eight seconds for each sample. A query to the reverse mapping is typically below a couple seconds, however, it does not scale well with dimensionality. With higher dimensions, the reverse mapping is not fast for the user, and optimization or analyzing sub-portions of the configuration space should be considered as alternatives. Therefore, AMF is accurate and efficient.

In conclusion, the results show that AMF satisfies many of these constraints and satisfies the major goal of bridging the intuitive gap between agent-level configuration parameters and system-level property values.

10.1   Future Work

In the course of the research, a number of possible directions for future work have arisen. Each of the following subsections discuss a possible subproblem in ABM meta-modeling or extensions to AMF that could produce interesting results.

10.2   Extension: Specifying Ranges for System-level Properties

One of the major problems with SCI is that queries can easily become overspecified. This is the case if the number of system-level properties exceed the number of configuration parameters. In the case of overspecification, the reverse mapping will not return any solutions, since they do not exist. To avoid this problem, SCI can be altered process ranges of system-level property values, instead of specific values. This provides some leeway and allows for more possibility of intersections. Instead of the solution of the reverse-mapping query being a hyperplane, it is now a hyperspace. The query plane used to intersect with the reverse mapping is also now a hyperspace, bounded by two hyperplanes.

This extension complicates the implementation significantly. In order to implement this extension in SCI, the equations used would be inequalities, complicating the calculation of the intersection. Any point that is satisfied by the set of inequalities over all simplexes could satisfy the system-level property ranges. In the rest of this subsection, the QT approach is described, but the implementation is left as future work.

The Quad-Tree (QT) approach for inverting the forward mapping is intended to be a simpler to implement approach than SCI. Also, specifying ranges for system-level properties is more natural in QT than in SCI. QT performs the same tasks as SCI, but instead returns a set of subspaces that must or could possibly contain configurations that satisfy the desired system-level property configuration. In general, a quad-tree is a tree data structure in which each node either has zero or four children. They can be used to iteratively segregate a two-dimensional space into several subspaces in order to give certain portions of the space more detail. Quad-trees use a notion of "black", "gray", and "white" cells: black cells represent a subspace in which all values are black, white cells represent a subspace in which all values are white, and gray cells represent a subspace in which some values are white sand some values are black. The benefit of using a quad-tree structure is black and white cells do not need to be expanded, as all their values are already determined. However, gray cells are broken down further by segregating its space into four children, which may be black, gray, or white. Grey cells can be broken down as many times as desired, but in general is capped at a certain depth, which I call the "granularity depth."

The idea of quad-trees can be used in the reverse mapping to approximate the solution space. Black nodes are ones in which all values within the subspace match the query, white nodes are ones in which none of the values within the subspace match the query, and gray nodes are ones in which some of the values within the subspace match the query. Instead of using squares to split the subspaces, QT must use hypercubes, as the configuration space is typically not two-dimensional. QT returns all the gray cells and black cells found by this

approach as an answer to a user's query.

Gray nodes are broken down iteratively until the granularity depth is reached. QT breaks down a hypercube (a pair of simplexes) by querying the forward mapping for the points needed to break a single n-dimensional hypercube into 2^n hypercubes (e.g., split a line into two lines, a square into four squares, a cube into eight cubes, etc.). Each new hypercube is then evaluated to see whether it contains the desired system-level property values or not, which can be determined by comparing the desired system-level property with the observed maximum and minimum among the corners of each hypercube. If the desired system-level property value is less than the maximum, and greater than the minimum, then possibly an intersection satisfying all system-level properties exists within this hypercube. If one of the values is not contained within this range, then the hypercube is marked as "white" and does not need to be expanded further.

This approach has the benefit that the intersections of hyperplanes do not need to be calculated, which may be difficult to implement. Although it is less accurate and the space it returns is not continuous, it serves the purpose of the reverse mapping in many ways. It still returns configurations that the user should use to generate the behavior and can still be visualized to show the nature of the configurations that generate a particular system-level property.

Another motivation for using QT over SCI is in specifying ranges for system-level properties is difficult to represent in SCI because all the equations are inequalities. Meanwhile, the implementation in QT is quite simple because either hypercubes contain the values, or do not. Details on the uses of ranges in querying the reverse mapping are discussed in Section 10.2.

The usage of QT on the fires domain is visualized in Figure 10.1. The thicker bars represent earlier separation. First, the space was split into the ranges 45–60 and 60–75. The system-level property ranges from .02 to .7 in the 45–60 subspace, so this space can

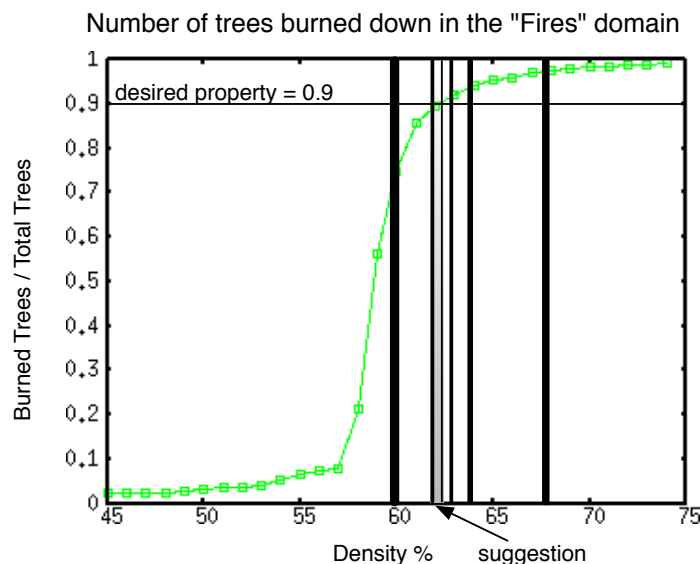Number of trees burned down in the "Fires" domain

FIG. 10.1. The subspaces generated by QT represent a range of configurations that are close to satisfying the desired system-level property.

be ignored in future divisions because it does not contain the value .9. The other half is subdivided at 67.5. This process continues five times, which is the granularity depth in this case. In a situation in which several solutions are possible, several subspaces will be returned as candidate configuration spaces.

To handle ranges of system-level property values, only minor modifications to QT must be done. The space is subdivided in the same way as standard QT, however, spaces that lie entirely within the ranged are marked as "black" and do not need to be subdivided further. Ranges marked as "white" do not need to be subdivided either. Gray areas are inspected more closely in order to increase the detail of the reverse mapping solution. A set of configuration spaces are returned that represent the configurations that will satisfy the system-level property range. This process is visualized in Figure 10.2.

The caveat with this approach is in non-monotonically changing domains, the maximum and minimum values at the corners do not necessary accurately describe the maxi-

Number of trees burned down in the "Fires" domain
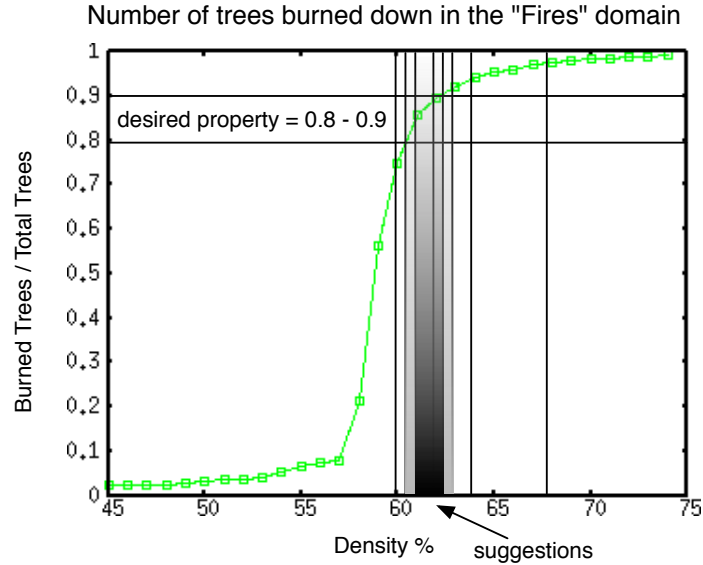
FIG. 10.2. The subspaces generated by QT represent a range of configurations that are close to satisfying ranges of the desired system-level property.

mum and minimum within the hypercube. If there exists a local minima or local maxima within a cube, the feature will be ignored. To avoid this problem, the starting grid of hypercubes should be sufficiently detailed.

10.2.1 Extension: Adaptive Meta-models

In some agent-based models a hidden property may continue to change. A hidden property is a feature of the environment that changes the behavior of the agents in some way, but is not directly detectable. In the case that the hidden property does not change, the learned mappings will adapt to this hidden variable and the mappings will continue to be accurate. However, in cases in which the hidden property changes over time, the learned mappings must be adaptive, as the value of the hidden property is not part of the configuration vector. Because of a changing hidden property, the system-level behavior of a system can change over time, yet be still running the same configuration.

Wind in a flocking ABM serves as a good example of this phenomena. A strong wind can change the behavior of a flocking system to be less cohesive. However, the value of the wind is not predictable, which can cause predictions about the system to be erroneous.

To tackle this problem, the meta-models built by the forward and reverse mapping must be adaptive to the current conditions in the ABM. I propose that an online optimization technique that incrementally adjusts the behavior of the system to compensate for hidden changes in the system. A continuous stream of current system-level property values will be going into the framework. The forward mapping will predict what should be happening with this configuration and is compared to the actual system-level behavior. The distance between the predicted and actual is minimized by incrementally changing the configuration in order to minimize this gap. Over time, the difference between the predicted and actual value will converge to zero.

The approach described here is an optimization approach, but is different from standard optimization because the initial starting position provided by the forward mapping is presumably close to the optimal configuration. Also, the derivative of the mapping can be used in a gradient ascent approach, in which the derivative is calculated from the forward mapping. Hidden variables typically will not change the nature of the system, only the specific values. That is, increasing one configuration parameter is likely to have the same sort of effect, but not exactly.

10.2.2   Correlated System-level Properties

One of the major assumptions used for the AMF approach to learning the reverse mapping is that the system-level property values are not correlated. This allows the reverse mapping problem to be split into a number of reverse mapping subproblems (one per system-level property). However, if the properties are correlated, the result of the reverse mapping may be inaccurate.

For example, consider two system-level properties a and b are correlated such that $a \cdot b^2 = 1$. Presume that AMF, while solving the reverse-mapping problem, averages a and b separately for the following two instances: $a = 100, b = \frac{1}{10}$ and $a = 400, b = \frac{1}{20}$. The averages are $a = 250, b = \frac{1}{15}$, however, $250 \cdot \frac{1}{15} \neq 1$, which clearly is not a valid instance.

To avoid this problem, a multi-variate learning approach must be taken. The forward mapping must be learned with a multi-variate regression algorithm, which must then be inverted in a multi-variate manner, as well. This type of approach will consider all properties at once at be immune to this problem.

10.2.3 Handling High Amounts of Dimensions in Simplical Complex Inversion

In Chapter 8, the five-dimensional configuration space of the Wolf Sheep domain proved to be too large for simplical complex inversion. I have considered a few approaches to tacking this problem in future work.

The first option is to use optimization instead of building a mapping. This approach has the major problem that it will not return a space of solutions—it will only return one. In many situations, this will be acceptable if the user is attempting to find a satisfactory configuration that will generate a specific system-level behavior. An interesting point to note is the behavior spaces are typically continuous. Therefore, if there are many configurations that will satisfy the particular system-level property specification, they will probably exist near the point found with optimization. A hillclimbing approach will move along these ridges of equal fitness and could return several possible configuration points. This will work particularly well in situations in which the solution configuration space is linear, because the optimization simply follows a line. However, with higher dimensional configuration solution spaces, the representation of a hyperplanar solution space would be difficult to develop.

Another approach to the problem would be to dynamically generate the majority of

the simplical complex at run time. This would allow a smaller portion of the mapping to reside in memory, making this problem far more tractable. A specific simplex can contains a desired system-level property if the system-level property is within the minimum and maximum values of the simplex's corners. These candidates can be broken up further to generate a more accurate mapping of the configuration solution space. The major difficulty in this approach is the existence of local minima and local maxima within a simplex. Consider the following example: a simplex has a minimum system-level property value of 4 and a maximum system-level property value of 6. The value being sought is 7. It is quite possible that at some point in the forward mapping, the value of the system-level property reaches 8, then decreases back down to 7 at the edge of the simplex. It is impossible to determine that this is the case from just the values of the simplex corners. One way a local maxima (or minima) could be inferred to exist within a simplex is to approximate the derivative (i.e., rate of change) of the system-level property going into the simplex. For example, if at all edges, the system-level property is increasing, then it is highly likely that a system-level property local maximum exists within this simplex. The derivative can be approximated by viewing the values of other knots nearby, or sampling additional points to approximate the derivative. The domains I sampled and many of the domains discussed in Chapter 9 do not exhibit behavior spaces with many local minima and maxima. Typically, the system-level property increase monotonically or has a single maximum, as the configuration changes. Therefore, this type of approach in approximating the derivative would probably be successful, since there are typically only a limited number of maximums.

Although many approaches can be applied to reduce the computational complexity of solving the reverse problem, most approaches will almost suffer the curse of dimensionality, along with SCI. As more dimensions are added, optimization techniques will have to search more of the space and SCI-type approaches will require more subspaces. Even approaches similar to non-linear regression, which can be functionally inverted, become

more complex with more dimensions. With NLR, more model parameters and more variables make the system of equations significantly more difficult to solve. Regardless of scaling issues, any improvement of performance in solving the reverse-mapping problem will allow researchers to inspect and analyze more complex agent-based models.

10.2.4 Optimization of a System-Level Property

In some cases, researchers may not want a configuration that produces a specific system-level behavior, but instead produces "the best" system-level behavior. In this case, an optimization approach, similar to that in work by Stonedahl and Wilensky (2010), could be used to find an optimal behavior. A SCI-type approach would not be needed, because typically an "optimal" behavior will be a single point, and does not necessarily need to be represented as a hyperplane.

Using the forward mapping could greatly improve the performance of work similar to that of Stonedahl and Wilensky, since instead of interacting with the ABM directly to calculate the fitness function, the optimization algorithm would be interacting with the forward mapping. This will greatly reduce the computation time of a particular optimization, at the cost of spending a significant amount of time training the forward mapping. If many optimizations are to be performed, training the forward mapping will save time in the long run, since it can be used as many times as needed. Instead, in a traditional optimization approach, the ABM will have to be re-sampled every time, even if the space being searched is the same as previous search spaces.

10.3 Closing Thoughts

It is my hope that this dissertation spurs additional research projects and discussions in tackling the problem of more efficient experimentation and deeper analysis of agent-based

models. This dissertation not only served as documentation for my particular approach and implementation, but also defined a number of core problems in this field. Many alternative implementations are possible, some of which have been outlined in the Future Work section of this chapter. Researching these additional solutions will lead to the discovery of new advances in the analysis of agent-based models. Additional tools and theory regarding analysis of agent-based models will improve their usefulness in current models and their applicability to newer, more complex systems.

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