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A Survey of Methods for Data Inclusion in System Dynamics Models: Methods, Tools and Applications

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A Survey of Methods for Data Inclusion in System Dynamics Models

Methods, Tools and Applications

James Houghton, Michael Siegel, Anton Wirsch, Allen Moulton, Stuart Madnick, Daniel Goldsmith

In 1980, Jay Forrester¹ enumerated three types of data needed to develop the structure and decision rules in models: numerical, written and mental data, in increasing order of importance. While this prioritization is appropriate, it is numerical data that has experienced the most development in the 25 years since Forrester made his enumeration. In this paper, we'll focus on how numerical data can be incorporated into models when written and mental data are known, and survey the techniques for doing so.

Motivation and Purpose

Numerical data is experiencing a renaissance because 1) traditional data such as census and economic surveys are more readily accessible 2) new sensors are measuring things that have never been measured before, and 3) previously 'unstructured' data - such as raw text, audio, images, and videos - is becoming more amenable to quantification².

Because of this explosion and the popular buzz surrounding 'Big Data', clients expect to see strong incorporation of data methods into dynamic models, and it is imperative that System Dynamics Modelers are fully versed in the techniques for doing so.

The SD literature contains surveys (Peterson 1976³ and Eberlein 1985⁴) that explain methods for including data in system dynamics modeling, but techniques have continued to develop. This paper attempts to bring these surveys up to date, and serve as a menu of modern techniques.

Structure

The paper is structured to follow the modeling process laid out by John Sterman in 'Business Dynamics'⁵: 1) Problem Articulation and Boundary Selection, 2) Formulation of a Dynamic Hypothesis, 3) Formulation of a Simulation Model, 4) Testing, 5) Policy Design and Evaluation.

Within each major step we discuss specific modeling tasks and relevant data techniques, and give a brief overview of the mechanics of that technique. We refer the reader to seminal works and good tutorials for further learning. Where appropriate we list some of the major software packages that support each technique. We show how the technique can be used specifically in the modeling task, with examples drawn from System Dynamics and related literature.

Scope

This is clearly not an exhaustive list of data techniques that could be applied to System Dynamics. Instead, we survey the techniques that have precedent in the SD literature, and draw support from outside traditions.

We choose only to touch on the parts of the model building process that show clear promise of benefitting from numerical data. We choose not to investigate methods of data collection or elicitation, which are covered elsewhere⁶.

1 Problem Articulation and Boundary Selection

The first and most important model-building step is to clearly identify the purpose for a model and the problem that it hopes to solve. This step requires investigation of the dynamic behavior of the system and its problem symptoms, and determination of the appropriate scope and resolution of the model. Randers explains this step in the classic 'Guidelines for Model Conceptualization'⁷; Mashayekhi and Ghili⁸ discuss problem definition as an inherently iterative process. From this section we omit qualitative tasks: phrasing the research question, description of problem behavior, and choice of model structure boundary, in order to focus on tasks with a strong data dependency.

1.1 Identify Reference Modes

A modeler should be able to identify the symptoms of problem behavior in the time-series data that the problem system generates. The process of identifying these reference modes is described well by Saeed⁹ and VanderWerf¹⁰.

Finding reference modes within time-series data is not always straightforward, and may require the modeler to look at the data in a variety of ways before the behavior becomes clear.

1.1.1 Exploratory Data Analysis and Data Visualization

Exploratory Data Analysis refers to visualization and statistical summary techniques that are designed to give the modeler an intuitive understanding of the nature of the data.

Description

Visualization methods generally show how a parameter of interest varies according to an independent attribute (time, geography, property, or relationship). Summary statistics can investigate the relationship of data with itself, by looking at averages, variances, and correlations.

Among others, Tukey¹¹ promoted Exploratory Data Analysis for development of intuition about data; in the years that followed, data visualization and summary statistics have become an integral part of introductory statistics courses, and are an ongoing area of research. Tufte¹² provides the quintessential resource for visualization of quantitative information, and Yau¹³ gives an introduction to modern techniques and tools. Keim¹⁴ discusses visualization as a form of Data Mining.

The vast majority of data or numerical analysis software suites provide some form of summary statistic and data visualization capability: Python(NumPy¹⁵, Matplotlib¹⁶, Bokeh¹⁷), R(native), Javascript(D3¹⁸), Matlab¹⁹(native), Gnuplot²⁰, etc.

Application to Reference Mode Identification

To identify behavior modes, the modeler needs to have a good understanding of the dynamic behavior of the system. Exploratory Data Analysis in the form of visualization and simple summary statistics allows the modeler to form that intuition by presenting numerical data in human-digestible formats. These formats allow the modeler’s eyes to look past noise to see the variety of growth, decay, or oscillatory modes that constitute the behavior of interest. Khan, McLucas and Linard²¹ use a variety of visual and aggregation methods to develop reference modes for the salinity of the Murray Darling basin.

1.1.2 Frequency Spectrum Analysis

Frequency Spectrum Analysis allows the modeler to see the strength of each of the oscillatory modes in her sample data.

Description

It is not uncommon to think about time-series data as being composed of a number of oscillations at different frequencies superimposed on one another. Fourier transforms are used to estimate the relative contribution of each of these oscillatory modes to the measurements. Fourier transforms come out of the signal processing community, with a seminal paper by Cooley and Tukey²², and a good overview of the method by Duhamel²³.

Software packages that support Fast Fourier Transforms and Frequency Spectrum Analysis include Python (Numpy.fft²⁴), R (Stats.spectrum²⁵), Matlab²⁶ (fft), and Excel (Analysis Toolpack)

Application to Reference Mode Identification

Frequency Spectrum Analysis can reveal the dominant modes of oscillation, and help the modeler identify the frequency band that captures the behavior of interest. Arango and Moxnes²⁷

demonstrate the use of Spectral Analysis to identify cyclical behavior in energy markets, as can be seen in Figure 1.

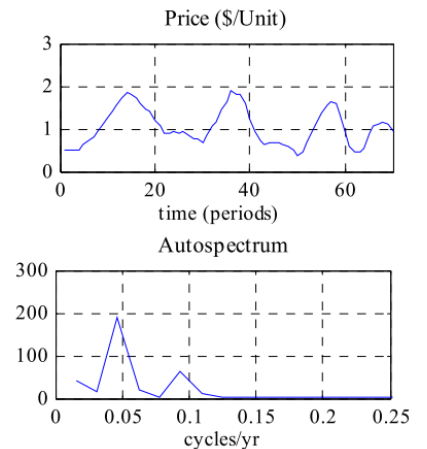


Figure 1: Market Price History and Spectral Density in Arango and Moxnes²⁷, showing two major oscillatory modes.

1.1.3 Phase Portraits

A phase portrait factors out the time component of a model to show how a pair of system components vary with respect to one another. The shape of the phase portrait curves can show if one variable is driving another, or if they oscillate in-phase or opposed to one another. A phase portrait can show if oscillations are being damped or becoming unstable, if the oscillations follow a standard pattern, or if the system is exhibiting chaotic behavior.

Description

A phase portrait is a set of curves whose x coordinate is described by the values of one variable of interest, and the y coordinate described by another. A phase portrait may show the direction of the flow in this space when the system is initialized with a variety of values for each parameter.

Phase plane analysis is frequently used in the Control Theory and Complexity Theory traditions. A number of texts provide introduction to phase plane analysis. See Chapter 2 in Enns and McGuire²⁸, Chapter 2 in Tien²⁹, and Tseng³⁰. Most plotting tools can create a phase portrait, although some provide more established mechanisms for doing so, including Python (PyDSTool³¹), and Matlab²⁶ (ppplane).

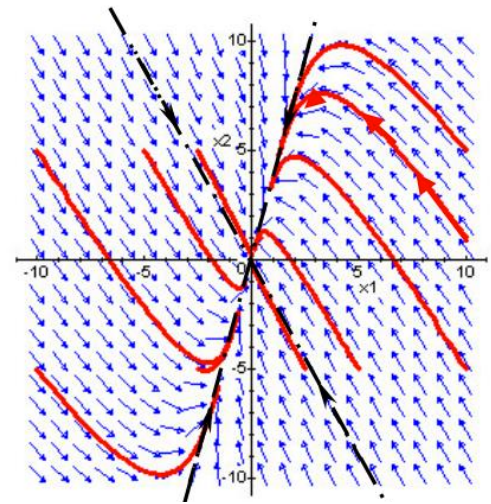


Figure 2: Phase plane demonstration of second order system in Guneralp³².

Application to Reference Mode Identification

Phase portraits can be useful tools in determining behavioral modes and dynamic causal influence. When phase plots show cyclic behavior the modeler can expect to see second order structure driving the model. When the motion of stocks is well correlated, she should look for a behavior that drives both, and so forth. Guneralp³² demonstrates the use of phase portraits to understand the dynamic behavior of a variety of simple system structures, as can be seen in Figure 2.

1.2 Infer Appropriate Aggregation Levels

System dynamics depends on the ability to aggregate individual actors or elements into groups whose behavior can be modeled as a unit. These groups may be based upon age, location, or other characteristics that define the group and its expected behavior. Rahn³³ describes how the process of aggregation can make stochastic behavior into analytically tractable flows, and takes a good look at this essential component of System Dynamics modeling.

In many cases there will be a natural set of choices for levels of aggregation, or a standard for doing so. For instance, students may be aggregated by grade, or into Elementary, Middle, or High School. When such a clear-cut distinction is not available, clustering algorithms can be used on the dataset to determine groups.

1.2.1 Machine Learning Clustering Algorithms

Description

Clustering algorithms work to identify sets of data-points in which the difference in attributes between members of each group is minimized, and the difference between groups is maximized. There are a variety of clustering algorithms that produce different

types of clusters. Clustering Algorithms come out of the Artificial Intelligence community, and a survey of these algorithms is provided by Xu and Wunsch³⁴.

Software packages that provide clustering algorithms include Python (Scikit-Learn³⁵), R (various packages), Matlab (Statistics Toolbox)

Application to Data Aggregation

In situations where intuitive or standardized methods of aggregation are infeasible, the modeler may choose to use a machine learning algorithm to identify cohorts based upon their shared attributes. Onsel, Onsel, and Yucel³⁶; and Pruyt, Kwakkel, and Hamarat³⁷ discuss clustering of behavior modes, although direct clustering for aggregation remains to be demonstrated in SD literature.

2 Formulation of Dynamic Hypothesis

In the second stage of model building, the modeler begins to determine the structure of the model in a largely qualitative way. Inferring the overall structure of a model based upon data is challenging, although there have been some attempts to do so. Data methods can be more helpful in an iterative modeling process where the structure of a new model may be based upon previous similar models, and the inference task is to infer which of a set of previous models best represents the current data. We omit here causal mapping of the system as this is the step in which the modeler begins to add written and mental data to the model, and as such is less of a numerical task. We also omit the creative and intuitive task of actual hypothesis generation.

2.1 Model Selection

In some cases there may be disagreement about the general structure of the system, as different parties have different mental models of the way the system works. If simple versions of these mental models are specific, data methods can be used to determine the relative likelihood that each model structure could be responsible for creating the observed data. The relative likelihoods of the model without respect to parameters are calculated as 'Bayes Factors'.

2.1.1 Markov Chain Monte Carlo

Markov Chain Monte Carlo (MCMC) can be used to infer the distributions of input parameters to a model when the output behavior of the system is known through measurement. In model selection, MCMC assumes the choice of model to be the parameter of interest.

Description

MCMC chooses a random set of parameters from 'prior' input distributions, executes a system model (which must have a stochastic component), and then calculates the likelihood of the observed data given the run of the model and the chosen input parameters. The algorithm uses this probability to decide whether to include the chosen input parameters in a posterior distribution. Repeating this process on the order of tens or hundreds of

thousands of times, distributions for the input parameters can be summarized using histograms or other density estimation methods.

Markov Chain Monte Carlo was developed to support nuclear engineering; and the primary algorithms used in MCMC were developed by Metropolis³⁸, Hastings³⁹, and Geman and Geman⁴⁰. Andrieu, Freitas, Doucet and Jordan⁴¹; and Brooks⁴² give good introductions to use of the technique. Software packages that provide MCMC algorithms include Python(PyMC⁴³), BUGS⁴⁴, winBUGS, R(MCMCpack), Vensim.

Application to Model Selection

A modeler can use Markov Chain Monte Carlo to help choose between multiple competing models. To do so she establishes a categorical variable that can take values corresponding to each of the candidate models. In each MCMC run, a value (and thus a model) is selected and the likelihood of the data given that model computed. After MCMC convergence, the relative likelihood of each model is proportional to the number of times its categorical variable value was selected.

Andrieu, Djuric and Doucet⁴⁵ expand on their introduction to MCMC with a description of how the method can be used to choose between models.

2.1.2 Bayes Factors

Bayes Factors serve as a relative likelihood of the validity of two models. While they won't tell the modeler that a particular model is correct, they will tell her if one model is a better representation of the measured data than another model.

Description

The Bayes Factor lets a modeler abstract the model from its parameters by calculating the likelihood ratio of the two models under any set of parameters that each model takes as valid. This takes the form of an integral of the likelihood over the parameter space. As this is often a large multidimensional integral, the modeler can use a sampling technique such as Markov Chain Monte Carlo to approximate its value.

Bayes Factors come from the statistics tradition and were first articulated by Jeffreys⁴⁶. Kass and Raftery⁴⁷ give an overview of the technique in its modern form. Software packages that specifically facilitate the calculation of Bayes Factors include Python (PyMC⁴³), and R(BayesFactor).

Application to Model Selection

Bayes Factors give weight to the preference one model should receive over another, and thus give a measure of confidence in deciding to reject one model in favor of its competitor. Alternately, the Bayes Factor may tell the modeler that there is no clear preference for one model over the other, and that some form of averaging, or a new model altogether, would be the preferred solution.

Raftery⁴⁸ demonstrates the use of Bayes Factors for model selection on social research. Opportunities exist for demonstrations of this technique in the SD literature.

3 Formulation of Simulation Model

Data methods can be extremely helpful in completing dynamic models whose structures have already been identified. The modeler can use these methods to help select equations to represent the relationships between system components, identify values for model parameters and initial conditions, and prepare exogenous inputs. Here we omit partial models and other methods of slicing the model before inference, as they are well established within System Dynamics and are not themselves data methods.

3.1 Identify Equations to Represent Relationships Between Variables

When a stock and flow structure has been constructed, the next step is to implement the equations that govern each relationship. In some situations the modeler can work from first principles, or infer scaling laws and nonlinearities from intuition. In other situations, she may have little understanding of how variables relate to one another and must infer the nature of the relationship from data.

3.1.1 Structural Equation Modeling

Structural Equation Modeling (SEM) attempts to infer relationships between a latent or unobserved variable and a number of observed variables. These latent variables may be estimators for a 'soft' quantity (such as 'morale') which itself may be further used in the model.

Description

SEM tries to fit the covariance matrix of a predictive model to the covariance of the observed parameters. Wright⁴⁹ provided the seminal paper on Structural Equation Modeling. Ullman⁵⁰ gives a tutorial of the basics of SEM, using a substance abuse model as a motivating example. A number of books give more detailed introductions, consider Kline⁵¹, or Bollen⁵².

SEM is well represented in the psychology and econometrics traditions. Several statistical suites have developed packages for structural equation modeling, including R(SEM, OpenMX), and SPSS(Amos).

Application to Equation Identification

SEM is applied to System Dynamics modeling as a method for including 'soft' variables into feedback models, identifying the relationship between the unobservable variable and additional observable characteristics.

Medina-Borja and Pasupathy⁵³ demonstrate the use of SEM in the context of a customer satisfaction and branch expansion model for a bank. Roy and Mohapatra⁵⁴ use SEM in a model of research and development laboratories.

3.2 Identify Influential Parameters

In parameterizing the model, it's likely that some parameters will have a strong influence on the outcome of the model, and others less so. If a modeler can identify these, she can prioritize the effort given to measuring each parameter value.

3.2.1 Sensitivity Analysis

Sensitivity analysis (also called Experimental Uncertainty Analysis or Propagation of Error) is a method for determining the impact of small changes of a system input parameter upon the computed output of the system.

Description

Sensitivity analysis uses numerical means such as Monte Carlo Analysis (see Section 4.2.1) to propagate errors or uncertainties in model parameters through to the model output. It is often performed one parameter at a time, and the relative magnitude of change between the input and output compared with that of other parameters. It can also be performed for multiple parameters simultaneously to determine the nonlinear interactions between parameters on the output.

Helton, Johnson, Sallaberry and Storlie⁵⁵ give an overview of sampling-based methods for sensitivity analysis in which they step through the various stages of the process: defining input distributions, designing samples of those distributions and executing the model, and reviewing the outcome; with a motivating example from industrial engineering.

Basic sensitivity analysis can be performed by any software capable of performing Monte Carlo Analysis, although a few packages have been developed to implement more advanced Sensitivity Analysis algorithms: Python(SALib⁵⁶), R(Sensitivity), Matlab(Control System Toolbox).

Application to Influential Parameter Identification

When sensitivity analyses are used in the model-building stage, the modeler is interested in finding the parameters with the greatest need for precision - these being the parameters for which a small error can lead the model to different conclusions. For each parameter, the modeler can calculate how tight the error bounds must be such that its relative contribution to the model uncertainty matches that of the other parameters.

Sharp⁵⁷ discusses methods of sensitivity analysis specifically in the System Dynamics setting. Powell, Fair, LeClaire and Moore⁵⁸ use sensitivity analysis to identify crucial parameters in an infectious disease model, and Hekimoglu and Barlas⁵⁹ apply the method to several business management problems.

3.2.2 Statistical Screening

Statistical Screening is a method of performing sensitivity analysis in system models that are computationally expensive, and it is infeasible to take a large number of samples.

Description

Screening looks at the correlation between variables and output values, instead of looking at the standard deviation of a number of samples when input values are varied. Welch et al⁶⁰ write an influential paper describing the process of statistical screening.

Application to Influential Parameter Identification

Statistical screening is important to the field of System Dynamics for its ability to identify and prioritize data collection and parameter estimation tasks. Ford and Flynn⁶¹ demonstrate the use of statistical screening to identify influential parameters in SD models, with examples of sales vs. company growth, and the World3 model. Taylor, Ford, and Ford⁶² demonstrate screening for application to a diffusion model and a rework model.

3.3 Summarize Measureable Parameters

In the ideal case, parameters of the model correspond to unique, observable characteristics of the real system. The task of preparing measurements of this characteristic for inclusion in System Dynamics models involves summarizing disaggregate sample data into single values or distributions that represent the true distribution of the concept in the system. Graham⁶³ gives an overview of this process, along with some traditional techniques for doing so.

3.3.1 Bootstrap Resampling

Resampling with bootstrap allows the modeler to estimate the error in the parameters of a probability distribution, based upon a finite number of observations of that distribution. (Note that statistical bootstrapping is distinct from bootstrap aggregating in machine learning.)

Description

Bootstrapping works by taking a subset of the sample data, and computing the parameter of interest (mean, median, etc.) for that subset. Repeating this process a large number of times can give confidence bounds for the likely values of the parameter in the sample data set, which are comparable to the bounds on the true population.

The bootstrap method comes from the statistics tradition, and was first introduced by Efron⁶⁴; Henderson⁶⁵, and Diaconis and Efron⁶⁶ provide tutorials and perspective on the method and its variants. A variety of software packages facilitate statistical bootstrapping, including Python (Scikit-Bootstrap⁶⁷), R (Boot⁶⁸), and Matlab (Statistics Toolbox).

Application to Parameter Summarization

Bootstrapping can be used to infer distributions for model input parameters such that those distributions can be properly used in subsequent Monte Carlo model testing. Dogan⁶⁹ describes this process specifically for the System Dynamics model parameter estimation setting, and demonstrate its use with examples from The Beer Game and quality erosion in the service industry, as seen in Figure 3.

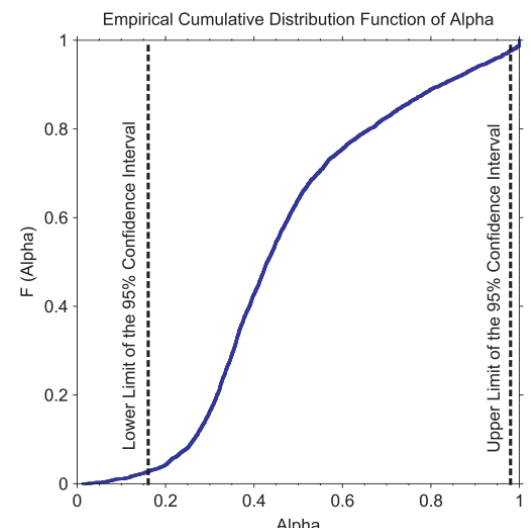


Figure 3: Dogan's⁶⁹ use of Bootstrap Methods to summarize parameters in a model of the Beer Game

3.3.2 Markov Chain Monte Carlo

For a description of Markov Chain Monte Carlo, please see section 2.1.1.

Application to Parameter Summarization

Markov Chain Monte Carlo can be used to estimate hyperparameters (such as mean and standard deviation) for a distribution representing a SD model parameter. In such a case, MCMC considers the data to be the product of a statistical model that takes the hyperparameters to specify an analytical distribution, and calculates the likelihood of the observed data. The MCMC algorithm then can be used to generate confidence intervals for the hyperparameters, which can be used as input to the simulation model.

3.4 Infer Unmeasurable Parameters

There are many cases in which parameter values cannot be directly measured, but based upon the model and its inputs and outputs, the modeler may be able to infer what the parameter values would need to be for the system model and the data to make sense together. She can perform this inference on either partial or full models, depending on the data that is available, using a variety of numerical techniques to yield either single values or distributions.

3.4.1 Regression

The concept of regression includes a variety of methods (Ordinary Least Squares, Orthogonal Distance, Ridge, etc.) for identifying the single best set of parameter values for a model, where 'best' is defined by some objective function, such as having the minimum square error between model predictions and system measurements.

Description

Most regression methods perform an optimization (see section 5.1.1) over the parameter space to minimize the difference between a prediction and system measurements. When applied to time-series data, regression is most effective for non-oscillatory behavior modes.

A variety of resources for learning regression methods exist; consider Ryan⁷⁰ or Vinod⁷¹. The vast majority of statistical packages and System Dynamics modeling software give some form of regression capability: Python (Scipy, Statsmodels⁷², Scikit-Learn), R(native), Matlab (Statistics Toolbox), Vensim, AnyLogic (Model Calibration), etc.

Application to Model Parameter Inference

Multiple regression is a common method for inferring values for unknown parameters in System Dynamics models. Higuchi⁷³ discusses parameter estimation using regression with an inventory model demonstration. Mayerthaler, Haller, and Emberger⁷⁴ use regression to parameterize a land use and transportation model.

3.4.2 Markov Chain Monte Carlo

For a description of MCMC, see Section 2.1.1.

Application to Model Parameter Inference

MCMC can be used to estimate a distribution for unknown model parameter values if the output of the simulation model is specified to represent the parameters of a statistical distribution. In this case, parameters can be sampled by the MCMC algorithm and the likelihood of data given the sample parameters computed. The MCMC algorithm traverses the parameter space, sampling from a distribution representing the likelihood that each parameter takes on a certain value. Osgood⁷⁵ describes the use of Markov Chain Monte Carlo for SD model parameterization.

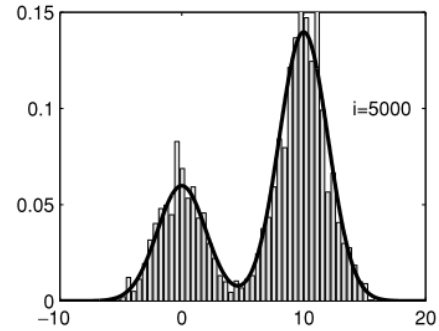


Figure 4: Inference of Distributions with MCMC in Andrieu, Freitas, and Doucet⁴¹.

3.4.3 Kalman Filtering

Kalman filtering gives an efficient method for calculating the unknown state of a system given a set of noisy measurements.

Description

At each time-step, a Kalman Filter uses a System Dynamics model to predict the current state of the system based upon its estimate of the previous state. It then combines its prediction with a measurement of the state (or components of the state) based upon its relative confidence in each.

Kalman filters were developed in support of the Apollo program, and come from an Aerospace and Control Theory background. Kalman's original paper⁷⁶ lays out the basics of his filter, and Du Plessis⁷⁷ gives a very readable introduction in 'The Poor Man's Explanation of Kalman Filtering', only a few years later. Awasthi and Raj⁷⁸ give a modern survey of the filter's modern variants.

Kalman filters are available within a number of numeric tools, including Python (Pykalman⁷⁹), Matlab(Simulink, DSP Toolbox), R(several, compared by Tussel⁸⁰), Vensim and others.

Application to Model Parameter Inference

In a parameter estimation setting, parameters can be considered as unchanging states for the Kalman Filter to infer. Examples of Kalman Filters applied to System Dynamics include Ryzhenkov's parameterization of an economic long wave model⁸¹, and Shiryaev, Golovin and Smolin's model of a one-commodity firm⁸².

3.5 Surrogate a Function

In some cases, two variables exhibit a well-defined relationship, but the form of that relationship is not well described by any simple functions. If these parts of the system are not the subjects of interest, the modeler may choose to surrogate the relationship with some form of piecewise model, or machine learning predictor.

3.5.1 Table Functions or Lookup Tables

Table functions give the modeler the ability to approximate a nonlinear relationship between one or more independent variables and an output variable.

Description

When an analytic representation of the relationship is complex or unavailable, the modeler constructs a table function using a set of points from that function, and these are interpolated between to find output values.

Lookup tables have been in use long before the advent of computers, and had previously been compiled to make trigonometric or logarithmic calculations simpler. Many software packages provide the basic data storage and interpolation function necessary to implement a lookup table, including Python(Scipy, Pandas⁸³), R(Stats), matlab(native), Vensim, Anylogic.

Application to Surrogating Functions

When a relationship between variables is unknown or complex, a lookup table provides an intuitive way to include information about the relationship in a model. Franco⁸⁴ presents a thorough introduction to table functions as they have historically been used in SD modeling.

3.5.2 Neural Networks

Neural Networks have the ability to encode multidimensional nonlinear relationships based directly upon training data, and to approximate a response to novel input that is consistent with the nonlinear relationships it encodes.

Description

Neural networks use training data to establish the relative weights of a set of links between neural nodes, these links encoding the relationships present in training data. Test data forms the inputs to these models, and their interaction with the established links provides the output.

Neural networks are a product of the Machine Learning community. McCulloch and Pitts⁸⁵ developed the first concepts of Neural Networks well before they were implemented on computer. Holena, Linke, Rodemerck, and Bajer⁸⁶ use neural networks directly for surrogating functions based upon data. Software capable of encoding neural networks includes, Matlab(NN Toolbox), Python(NeuroLab⁸⁷, PyBrain⁸⁸), and a number of standalone packages.

Application to Surrogating Functions

System Dynamicists can use neural networks in place of table functions, especially in situations with complex, multidimensional relationships that must be estimated from data. Alborzi⁸⁹ demonstrates the use of a neural network to approximate a function, using the example of gravitational attraction between two bodies.

4 Testing

After the model is built, the next task is to build confidence in the model's ability to represent the real system. Here the modeler can use data for its ability to disprove the model, show where its weaknesses are, and determine how she can improve it. In each case the modeler is looking at the model's ability to predict the data in a given set of conditions, and to test the model's robustness to different types of errors. Forrester and Senge⁹⁰ give a definitive guide to System Dynamics model testing. Barlas⁹¹ elaborates with a procedure for conducting various forms of model testing.

In this section we omit qualitative tests, such as tests for boundary adequacy, and dimensional consistency; numerical tests with little reliance on data (beyond model calibration): test of conservation laws, extreme conditions, loop knockout, and surprise behavior tests. These omissions help us focus on the tests with strong data reliance.

4.1 Compare Point Predictions with Numerical Data

The most logical quantitative test of a predictive model is its ability to make predictions. When a model is calibrated with best-fit parameter values, it is only able to make point predictions, which are unlikely to follow the true behavior of the system exactly. A modeler can look at the difference between the model prediction and the observed behavior in both the time and frequency domain for various parts of the model and various sections of the data.

4.1.1 Summary Statistics

Summary statistics aggregate the difference between a model point prediction and the observed value, according to some weighting function. These can be decomposed into components due to bias, variance, and covariance.

Description

Summary statistics include variants on Mean Square Error, the Coefficient of Determination, Theil's U statistics, and others. Sterman⁹² describes the appropriate use of summary statistics for System Dynamics models. Oliva⁹³ shows how these metrics are calculated using Vensim.

The majority of statistical packages are capable of calculating basic summary statistics: Python(Scikit-Learn, Statsmodels), R(Metrics), Vensim.

Application to Point Prediction Assessment

Summary statistics are used to estimate the goodness of fit of a model to historical data. System Dynamics models are often interested not in the magnitude of the total error, but in

the way that error is composed. By using a variety of summary statistics a modeler can determine if the error in her models is relevant to the purpose of the model. As an example, Stephan⁹⁴ uses summary statistics to build confidence in models of software development.

4.1.2 Cross Validation

Cross validation (or out-of-sample testing) works to improve confidence that the model represents the underlying behavior of the system, and that correspondence between the model and the observed data is not merely a result of over-fitting the model to the data.

Description

Cross validation works by breaking a dataset into 'training' and 'testing' components. The training set is used to parameterize the model, and the testing set is used to measure the ability of the model to make predictions. If possible, a modeler may choose to partition the data in a variety of ways and repeat the analysis.

When the system is time-dependent (as is usually the case with feedback models) and data is not significantly in excess of the relevant period of the system, there is a limited range of ways that the data can be meaningfully partitioned.

Cross validation comes from the statistics tradition. Picard and Cook⁹⁵ give a good overview of the use of cross validation to combat over-fitting in regression models. Software that facilitates cross validation includes Python (Scikit-Learn), R (A variety of packages summarized by Starkweather⁹⁶), Matlab(Statistics Toolbox) and others.

Application to Prediction Assessment

Cross validation in system dynamics can be challenging, as the complex time-dependent nature of the systems in question increases the difficulty of partitioning data into independent subsets. Randers⁹⁷ demonstrates out-of-sample testing in the qualitative comparison of predicted and measured wood pulp inventory and price.

4.1.3 Family Member Tests

Family Member Tests are a special form of cross-validation or out-of-sample testing, in which the modeler uses the model structure to predict the behavior of a structurally parallel but physically separate system. As with Cross Validation, Family Member Tests work to verify that the model fit is due to the structure of the system model, and not to a lucky guess of parameters.

Description

If appropriate family member systems are available, a modeler may choose to reoptimize the model based upon data from the family-member system in order to support the fidelity of the model structure and equations; or use the original parameter values to support the full data and modeling process. The modeler can then apply either point-wise or statistical measures to evaluate the model's predictive ability.

Family Member Tests are described by Forrester and Senge⁹⁰, and well elaborated by Sterman⁵(21.4.9).

Application to Prediction Assessment

System dynamics is principally concerned with identifying the structure of a system, and structural similarities between systems. These similarities allow a model developed in the context of one system to be applied to another, structurally similar system with few changes. Teekasap⁹⁸ tests a model of the economy of Thailand by evaluating its ability to fit data for the structurally similar Malaysian economy.

4.1.4 Frequency Spectrum Analysis

For a description of the method, see section 1.1.2

Application to Point Prediction Assessment

In systems with oscillation and noise, small changes in system parameters can lead to large deviation between model prediction and system observation after only a few periods. Spectral analysis, however, can reveal similarity between the strength of oscillatory modes excited in the model and the real system.

Eberlein and Wang⁹⁹ demonstrate the use of spectral analysis to evaluate the ability of a model to replicate behavior modes by comparing power spectral density of the predicted and observed behavior in the frequency domain region of interest.

4.2 Compare Statistical Predictions with Numerical Data

If models are calibrated with distributions of parameter values, the modeler can develop statistical predictions of output values. In this case, she can calculate the likelihood of the observed data given the assumption that the model is correct. The modeler uses statistical and graphical measures to determine how well the model fits the data.

4.2.1 Monte Carlo Analysis

Monte Carlo Analysis is helpful when the parameters of a model are given as statistical distributions, and we want to find statistical prediction (as opposed to a point prediction) of the output behavior of the system.

Description

Monte Carlo Analysis draws a set of parameters from a distribution of possible values, and uses those parameters to execute a dynamic model. The output is recorded and the process repeated on the order of tens of thousands of times. The collected output values are summarized using a histogram or other density estimation method to generate an expected distribution of the behavior of the system given each input distribution.

Monte Carlo Analysis was developed to aid in nuclear energy calculations by Metropolis, Rosenbluth, and Teller³⁸, and expanded and explained by Metropolis and Ulam¹⁰⁰. There are a variety of articles and books detailing Monte Carlo and its derivatives.

Most statistical packages are capable of performing Monte Carlo Analysis, and the basic techniques are not difficult to implement.

Application to Statistical Prediction Assessment

Monte Carlo Analysis gives the modeler the ability to propagate uncertainty in parameter estimates through to the model output. Well executed, the method can produce calibrated statistical forecasts of system behavior. Hagenson¹⁰¹ discusses the use of Monte Carlo techniques to study capacity for airfield repair. Santos et al¹⁰² apply the method to simulation of pulp prices. Moxnes¹⁰³ applies Monte Carlo Analysis to discuss decision making with regard to greenhouse gasses, and Phillips¹⁰⁴ discusses the use of Monte Carlo to ensure the robustness of model conclusions.

5 Policy Design and Evaluation

When a modeler is confident that her model sufficiently represents the system, and replicates its problem behavior, she begins to craft interventions to improve performance. This requires her to identify places in the system where she is able take action, and determine what type of action will have the desired effect.

From this section we omit the qualitative tasks of brainstorming model structural changes, and the tasks that require no new data techniques: testing for policy compatibility, robustness to model uncertainty, etc.

5.1 Explore Parameter Change Policies

When leverage points have been identified, a modeler can use some form of optimization to discover new values to drive parameters towards, respecting the costs of doing so.

5.1.1 Optimization

The term 'Optimization' covers a range of methods for choosing a set of input conditions that maximize or minimize a desired output state of a model.

Description

Many types of optimization exist, each with a variety of algorithmic implementations: slope following algorithms, edge condition assessment, stochastic methods, genetic algorithms and others. The best optimization for a specific problem depends largely on the topography of the reward function in parameter space. For a brief overview of optimization methods in the context of supply chain analysis, see Christou (Ch 2)¹⁰⁵. For a more detailed, modern introduction, see Chong and Zak¹⁰⁶.

Optimization is well established in Engineering and Applied Mathematics. Most computational environments include some form of optimization, several include Python(Scipy, DEAP¹⁰⁷), Matlab(Optimization Toolbox), R(native, GA), Vensim, and Anylogic.

Application to Policy Change Identification

The choice of a policy intervention in System Dynamics balances a number of factors, including performance, viability, and robustness. Optimization can be used to tailor strategies for peak performance subject to realistic constraints. Coyle¹⁰⁸ begins a

conversation about optimization methods for policy design in System Dynamics that is continued by Macedo¹⁰⁹. Graham and Ariza¹¹⁰ demonstrate the use of policy optimization in the context of market placement strategy.

5.2 Adapt Policy in Light of New Information

Frequently, the optimal intervention strategy is not to change a parameter or system structure once, but to respond dynamically to the state of the system continuously or in regular intervals. In these cases the modeler can draw from control theory and sequential decision theoretic approaches to plan her interventions.

Hamarat, Pruyt and Loonen¹¹¹ discuss the need and potential for adaptive, robust policy making based upon System Dynamics models.

5.2.1 Q Learning

Q Learning (or Reinforcement Learning, Approximate Dynamic Programming) is a method of sequential decision making which optimizes the balance of payoff in the immediate and future time, taking advantage of new information about state and uncertainties that becomes available as time progresses.

Description

Q-Learning solves a dynamic programming problem that computes the expected future payoff for a variety of possible future states, and suggests the optimal decision at each time-step based upon the assumption that optimal decisions will also be made in future states.

Q-Learning comes from the Machine Learning and Decision Theory traditions. It was first articulated by Watkins in his PhD thesis¹¹², and later elaborated in Machine Learning¹¹³. Cybenko, Gray and Moizumi¹¹⁴ give a tutorial and overview of the method. Several packages implement q-learning algorithms: Python(Reinforcement Learning Toolkit¹¹⁵), R(qLearn); a variety of other unpolished code examples are available.

Application to Policy Adaptation

Q-learning adds to System Dynamics modeling a programmatic method for structuring adaptive policies capable of dealing with uncertainty. Rahmandad and Fallah-Fini¹¹⁶ introduce the use of Q-learning and system dynamics models for adaptive policy development.

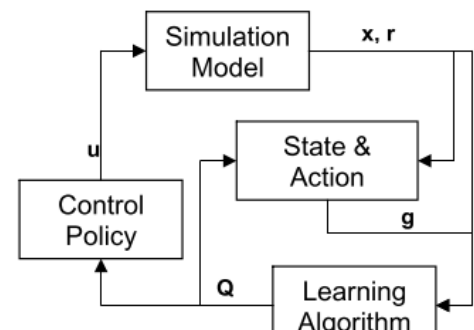


Figure 5: Learning and State Aggregation Process in Rahmandad and Fallah-Fini¹¹⁶.

6 Conclusion

In conducting this survey, we have identified a number of data techniques with potential to support System Dynamics that do not seem to be in common use. In *Problem Conceptualization*: Frequency analysis for time horizon and resolution determination. In

Model Formulation: Frequency domain regression, Indirect Inference and System Identification, model-based interpolation and filtering for exogenous inputs, Sequential Monte Carlo. In *Model Testing*: Brier Score, Reliability and Sharpness Diagrams. For *Policy Development and Verification*: Model-Predictive Control, virtual control groups, dynamic models for real-time system inference and monitoring.

The breadth of techniques for data inclusion in System Dynamics models, and the diversity of applications in which they can be useful mean that any survey of this type will be incomplete; and the rapid pace of new development means that there will soon be techniques to add to this list. Readers should continue to monitor developments in data mining, machine learning, and computer science to see how lessons from these fields can be brought to bear on dynamic models of complex systems.

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