An Evidence-Based Approach to Fidelity

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Abstract

We describe a new technique leading to quantifiable predictions during fidelity, validation, and verification processes. The technique described uses the structure of the theory under which a model or simulation is developed. We quantify the concept of evidence using odds. Experiments may lead to complex trees from which we can compute odds; the algorithms are based on our definition of inverse logic.

> "A habit of basing convictions upon evidence, and giving to them only that degree or certainty which the evidence warrants ... [would] cure most of the problems in the world." Bertrand Russell.

1 Introduction

We describe work in progress to develop formal methods and tools for verification and validation of models and simulations. Such tools would be useful if they could be integrated into the natural modeling and simulation development cycle and if they could lower costs and enhance quality without being too intrusive. We present a mathematical system based on the idea of *systems theories* and is a natural outgrowth of [18]. From the structure of the theory we can develop statistical measures that quantify the evidence.

Verification has a long history of computer tools. Fidelity, on the other hand, is relatively new issue. Fidelity (called *validation* in the sciences) is defined in [12] as

> "the degree to which a model or simulation reproduces the state and behavior of a real world object or the perception of the real world object, feature, condition, or chosen standard in a measurable or perceivable manner; a measure of the realism of a model or simulation."

In general, fidelity studies will require observations that have inherent uncertainty; simulations may interject uncertainty in many ways. Therefore, we expect reasoning with and about uncertainty to be a major issue in fidelity studies. Validation, as defined in [12], is concerned with both fidelity models and the setting of statistical parameters.

Reasoning with and about uncertainty has a long history. Probability and the scientific method hark from the 17th Century. More recently, artificial intelligence research have produced whole theories of uncertainty (see [17]); *A Mathematical Theory of Evidence* by Shafer [16] and Pearl's *Causality* [13] deserve special mention. In other formal method approaches, program proofs [1] and model checking [5] are other possible approaches to understanding uncertainty.

Unfortunately, most approaches to dealing with uncertainty require certain probabilities to be available; how to do this is controversial. We focus on one new approach to computing such probabilities using the proof of the theorems as constraints on the probabilities.

We link our investigation to Sargent's new diagram, Figure 1. Notice that *systems theory* is the single entity that bridges the gap between the *real world* and the *simulation world*, making *system theory* central to modeling and simulation (M&S) as well as to validation, verification, and accreditation (VV&A). Since systems theories are the central issue, we must relate VV&A terminology to the systems theory paradigm (This is the subject of another paper). System theories are formal mathematical systems, but they can be used for planning and management of the development cycle. The system theory that is assumed by a model or simulation should determine measurable, objective conditions for fidelity and verification activities. Models are often special cases of a more general theory. Simulations can be models themselves or instances of models.

A ready example of a systems theory is linear optimal control theory of dynamical systems used in virtually every aspect of modern technology. The *domain* of the theory is any object that fits the *assumptions* of the theory as well as any mathematical *axioms* laid out. Generally, the objects of the theory fit some form of *behavioral* representation. The domain is chosen based on a *problem* to be solved. The output of the theory is a *justified, coherent* methodology for solving the system problem. This methodology generally concerns either the *analysis* of behavior or the *synthesis* of controls (or both). But the theory is formal, relying on properties that may not hold in the real world. Engineers have learned how to adjust for these situations; in a sense, engineers validate by prototype and test, but they are guided by the formal conclusions.

We chose *uncertain dynamic systems* as the general theory. Uncertain systems [15] were defined in 1973 with continuous development since. Uncertain systems recognize that we must *estimate* such variables as state and that *observations* are statistical. These must be linked by a mathematical model explaining the estimation and the error behavior. Let $\mathbf{x}$ be the true values of the state variable and $\hat{\mathbf{x}}$ be the estimated value. Let $\mathbf{z}$ be the actual observed value and $\mathbf{v}$ be the uncertainty in $\mathbf{z}$. The *estimation* problem for the theory is

> Given the a priori model for the uncertainty $\mathbf{x}$, $\hat{\mathbf{x}}$, and $\mathbf{z}$, determine a particular a posteriori model for the uncertainty of $\mathbf{x}$ which which involves the "least" uncertainty. [15].

An example of an uncertain system is the discrete time linear system with white noise

$$\begin{aligned}
\mathbf{x}(n\Delta + \Delta) &= \mathbf{\Phi}(n\Delta)\mathbf{x}(n\Delta) + \\
&\quad \Delta\mathbf{G}(\mathbf{n\Delta})\mathbf{w}(n\Delta) \\
E\{\mathbf{w}(n\Delta)\} &= \mathbf{0} \\
E\{\mathbf{x}(0)\} &= \mathbf{0} \\
E\{\mathbf{x}(0)\mathbf{w}'(n\Delta)\} &= \mathbf{0} \\
E\{\mathbf{x}(0)\mathbf{x}'(0)\} &= \Psi \\
E\{\mathbf{w}(n_1\Delta)\mathbf{w}'(n_2\Delta) &= \begin{cases} \Delta^{-1}\mathbf{Q}(n_1\Delta), & n_1 = n_2 \\ (0), & n_1 \neq n_2 \end{cases}
\end{aligned}$$

where $\mathbf{w}$ is a white noise process. Uncertain systems add a new problem: the *state estimation problem*. For the above system, the estimation problem can be solved with Kalman filters.

Section 2 develops a method of evidentiary reasoning based on the observed odds. Section 3 illustrates the method by exploring the fairness of a coin. The need to invert implication leads to Section 4 with an example based on the above uncertain system presented in Section 5. The simple approach in this last section must be augmented by more general methods outlined in Section 6. Conclusions and future work are presented in Section 7

2 Probability Theory as Inverse Logic

The goal of modeling is to produce a system theory concerning the objects of the theory. Such a theory is primarily logical in that the theory is justified through proof. These proofs produce the ability to justify various referents: measures of state or behavior predicted by the theory. Fidelity, and by subsumption, validation, seeks to quantify the degree to which the observed systems actually predict the referent values.

Let $\{H_1, H_2, \ldots, H_m\}$ be the hypotheses of the systems theory and $\{C_1, \ldots, C_n\}$ be the conclusions. Then the methodology and theorems of the theory link the two through a line of reasoning.

$$\frac{H_1, H_2, \ldots, H_m}{C_1, \ldots, C_n} \text{ (Methodology, Theorems)}$$

The fidelity question is the following. If we observe an object, say x, that satisfies the conclusions $C_j(x)$ what can we say about $H_i(x)$? Section 2.1 describes a formalization of the term *information*. Using that definition we define *evidence* in Section 2.2 and how to compute the collected evidence as a measure of fidelity. Section 3 provides a elementary example using an elementary probability example: Given a sequence of heads and tails from a coin, how can we judge the fairness of the coin?

2.1 Information

We begin with the concept of *information*. The term has several interpretations both formally (such as *information theory*) and informally. We build on the works of [7, 8, 10, 11, 14]. Information is a measure of our knowledge of the state of the system after an event relative to our overall knowledge of the state. It is a measure of relevance.

We first consider the *likelihood* function:

$$L(H : C|G) = \frac{P(C|H\&G)}{P(C|G)}, \tag{1}$$

where $L(H : C|G)$ is read "the likelihood of H in light of event C given global knowledge G." Normal use of the term *information* leads to the interpretation that if the likelihood is one, we would say there is no information:

$$I(H : C|G) = log_b L(H : C|G). \tag{2}$$

The base b of the logarithms is immaterial allowing us to use "natural" units, such as decibels and bits.

2.2 Evidentiary Reasoning

Following [7, 8], we want to measure the evidence available based on the information at hand. In our case, this is the difference in the information for a state minus the information available for not being in that particular state. In other words,

$$\begin{aligned} W(H:C|G) &= I(H:C|G) - I(\bar{H}:C|G) \\ &= \log_b \frac{P(C|H\&G)}{P(C|\bar{H}\&G)} \qquad (3) \\ &= \log_b F(H:C|G), \qquad (4) \end{aligned}$$

where $\bar{H}$ is the complementary state of H. Notice that W is naturally stated as "odds". Using Bayes theorem in its *odds* form we get

$$O(H:C|G) = O(H|G)F(H:C|G)$$

and the log odds as

$$\log_b O(H:C|G) = \log_b O(H|G) + \log F(H:C|G).$$

We take this to be our computational rule for *evidence*

$$\begin{aligned} e(H:C|G) &= e(H|G) + \log F(H:C|G) \\ &= e(H|G) + W(H:C|G). \end{aligned}$$

In order to make the summation start at zero, we agree that the evidence at the beginning of a study is zero by taking the initial odds to be 1.

3 Example

We choose a elementary probability problem to illustrate evidentiary reasoning: coin tossing of a fair coin. Coin tossing often shows up before either conditional probability or Bayes theorem are studied formally because our intuitions are generally easy to examine.

In our context we define

$P(Head\|Fair)$	$1/2$
$P(Tail\|Fair)$	$1/2$
$P(Head\|Unfair)$	$(1-2\epsilon)/2$
$P(Tail\|Unfair)$	$(1+2\epsilon)/2$

Mathematics has taken the "easy" direction: The experimenter takes a coin known to be fair and runs experiments. The validation question is harder: "Given a sequence of coin tosses, how can I decide whether or not the coin is fair?"

3.1 Development

In this example, it is easy to compute the factor directly

$$\begin{aligned} F(Fair:Head|G) &= \frac{P(Head:Fair|G)}{P(Head:Unfair|G)} \\ &= \frac{1}{2} / \frac{1-2\epsilon}{2} \\ &= \frac{1}{1-2\epsilon} \end{aligned}$$

On the other hand,

$$F(Fair:Tail|G) = \frac{1}{1+2\epsilon}.$$

ϵ can be between [0, .5]. If ϵ is zero, then the coin is fair and the sum of the evidence is zero. But if ϵ is 0.5, then any head is impossible and $F(Fair:Head|G) = \infty$ while $F(Fair:Tail|G) = 1/2$.

The weight of evidence is logarithm of the factor, so

$$\begin{aligned} W(Fair:Head|G) &= -\log(1-2\epsilon) \\ W(Fair:Tail|G) &= -\log(1+2\epsilon) \end{aligned}$$

If we use common logarithms, we are measuring evidence in *bels*; multiply by 10 and we get *decibels*, a measurement commonly used in engineering. The author generated 100 samples of 20 random numbers each from the binomial distribution with $p = 1/2$. This is the $\epsilon = 0$ case. The total evidence is the sum which turned out to be 30.58 (bels) for this sample set. That is, is 306 decibels a good number or a bad number? 306 is one chance in 10^{30} that the coin is not fair.

A second experiment using the same rubric was used. In this second example we intentionally choose a distribution that could not be a binomial: the log normal with mean 0.45 and variance 0.14. This is decidedly spiked around 0.45. In this case, the evidence was -618. Again, the evidence is off the chart, but as evidence against.

Result. We have shown that if we were to observe the first 2,000 trials we would most likely conclude that our theory is valid. The second set of 2,000 trials we would be forced to conclude that our theory was wrong or that we did not have a fair coin. Notice that we cannot conclude that the coin is unfair. Why is this?

4 Inverse Reasoning

Our conclusion comes from the laws of logic. While it is true that we can say "If $a \to b$ and a, then conclude b" it is also true that "If $\neg a$, then b. Since we are reasoning "backward" from the conclusions, we must deal with both situations.

George Pólya considered many of these concepts in [14]. To understand Pólya, we need to understand that Bayes Rule is an application of standard implication.

If $A \to B$ then

$$P(B|A)P(A) = P(A|B)P(B)$$

Since B is a consequence, the left conditional is 1.

$$P(A) = P(A|B)P(B)$$

Solving for $P(A|B)$:

$$P(A|B) = \frac{P(A)}{P(B)} \quad (5)$$

$$O(A|B) = \frac{P(\bar{B})}{P(B)} \quad (6)$$

$$(7)$$

In other words, if $A \to B$ and we observe B, then A is more plausible by the ratio of $P(A)/P(B)$. In odds terms, only B shows up.

5 Evidence Calculations in Static Uncertain System

A static model of uncertain dynamic systems is described by equations

$$\mathbf{z} = \mathbf{H}\mathbf{x} + \mathbf{v} \quad (8)$$

$$E\{\mathbf{x}\} = \mathbf{0} \quad (9)$$

$$E\{\mathbf{v}\} = \mathbf{0} \quad (10)$$

$$E\{\mathbf{x}\mathbf{x}'\} = \mathbf{\Psi} \quad (11)$$

$$E\{\mathbf{v}\mathbf{v}'\} = \mathbf{R} \quad (12)$$

$$E\{\mathbf{x}\mathbf{v}'\} = \mathbf{0}. \quad (13)$$

This represents the observation of a system that is static but the observation is uncertain. Using elementary probability considerations, we can show:

$$\cfrac{\cfrac{Eq8 \quad Eq9}{E(\mathbf{z}) = \mathbf{0}} \quad Eq10 \quad Eq11 \quad Eq12 \quad Eq13}{\mathbf{\Gamma}_z = \mathbf{H}\psi\mathbf{H}' + \mathbf{R}}$$

This presentation makes clear the relationships among the assumptions and the conclusions. The model also makes clear that there are only two possible observations: $E(\mathbf{x})$ and $\mathbf{\Gamma}_z$. Suppose now that these are measured with $O(E(\mathbf{z}) = 0) = d_1$ and $O(\mathbf{\Gamma}_z = \mathbf{H}\psi\mathbf{H}' + \mathbf{R}) = d_2$. What can we conclude about the odds of Eq 8 being true?

Using Eq 6 in odds form, we see that we have

$$d_2 = O(E(\mathbf{z}) = \mathbf{0}\&Eq10\&Eq11\&Eq12\&Eq13)$$

$$d_1 = O(Eq8\&Eq9)$$

If we adopt a "no information" principle then

$$O(Eq8|E(\mathbf{z}) = 0)) = \sqrt{d_1}.$$

For such a simple structure, this informal approach is adequate. What about the more complex cases likely to arise in practice?

6 General Solution

In the general case, the information presented by the systems theory and any proofs in that theory are likely to be very complex. It is generally true that proofs will define a tree [19] that can be used to generate information. This is a common approach in artificial intelligence. Perhaps the most complete version of the artificial intelligence approach is in Pearl [13]. However, the general approach traverses the tree in a forward direction — in the *verification* direction.

It turns out that George Boole devoted almost one-third of his famous book [2] to probability. Boole's goal was to develop methods by which any set of equations with any given set of prior probabilities could be solved for the remaining probabilities. Boole's methods were highly criticized during his lifetime; it would be more than a century for his method to be vindicated [9]. The thread of his ideas is now known as *probability logics*, among other names. Genesereth and Nilsson [6, Chapter 8] describe a general solution technique in Sections 8.3 – 8.7. Briefly, the general solution is to develop an optimization problem which describes the constraints on the probabilities of the system. We can then find an optimal solution. Since probabilities and odds are inter convertible by

$$p(Q) = O(Q)/O(Q + 1),$$

we can use the same technique to solve for the odds of any event. From this, we can determine the evidence needed for the validation problem at hand.

This technique offers an important advantage: it is adaptive. The basic process is:

1. Define the *graph* of the validation problem to be the proof tree described above.
2. Using the rules laid out by Boole, we can convert the graph to an optimization problem in *odds*.
3. Solve this optimization problem for the odds given the observations. The optimization problem can be augmented by cost and risk data.
4. Solve the evidence problem for this initial graph.
5. Iterate.

7 Conclusion — The Basis For Formal Methods

We have developed an approach to validation that is both logically sound and leads to quantifiable predictions. The graph of the application can be processed in either direction. The basic process is

1. The system theory under which the model or simulation is identified.
2. Questions concerning the model or simulation are developed by considering the proofs in the theory. Proofs can always be represented by a tree.
3. Questions concerning *verification* are processed in the from the assumptions and axioms toward the conclusions.
4. Questions concerning *validation* are processed *in reverse* using Boole-Pólya-style rules. This results in an optimization problems solvable by standard methods.

Work remains to be done in the complete specification of the inverse logic. For example, Bayes conditioning is not exactly the same as implication. From logic, the *definition* of implication is $\neg(A\&\neg B)$ which has a probabilistic rendering of

$$\begin{aligned} P(A \to B) &= 1 - P(A)P(\bar{B}) \\ &= P(\bar{A}) + P(B) - P(\bar{A}\&B). \end{aligned}$$

Work dealing with boolean equations [3] may contain algorithms to effectively compute such expressions.

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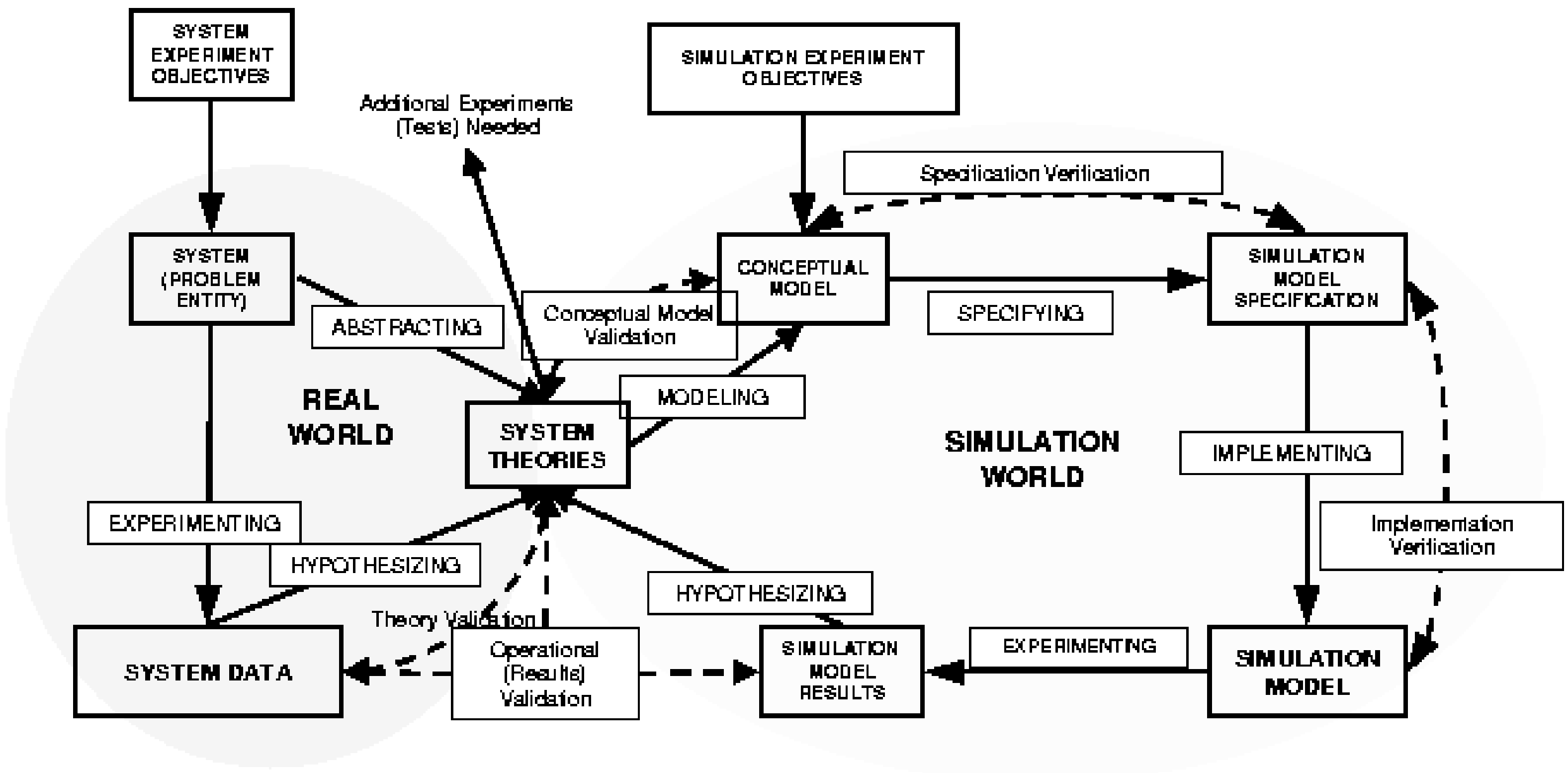
Real World & Simulation World Relationships in Developing System Theories and Simulation Models with Verification and Validation (V&V) -- additional explanation in annotation



Notes:

Experiment objectives should derive from validated requirements

Dotted red implies comparison, assessment, or evaluation

Validation is always relative to objectives/requirements/intended use

Diagram by Robert G. Sargent (Syracuse U) Jan 01