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Wavelet ANOVA bisection method for identifying simulation model bias

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ABSTRACT

High-resolution computer models can simulate complex systems and processes in order to evaluate a solution quickly and inexpensively. Many simulation models produce dynamic functional output, such as a set of time-series data generated during a process. These computer models require verification and validation (V&V) to assess the correctness of these simulations. In particular, the model validation effort evaluates if the model is an appropriate representation of the real-world system that it is meant to simulate. However, when assessing a model capable of generating functional output, it is useful to learn more than simply whether the model is valid or invalid. Specifically, if the model is deemed invalid, then what aspects of the model are incorrect? Is it possible to identify over what range the model data are a poor representation of the system data? Current V&V methods cannot identify these ranges. This paper proposes a wavelet analysis of variance (WANOVA) bisection method that first assesses model validity and can also identify the interval(s) over which the model is biased. The technique is illustrated using several simulation studies. Ultimately, this new method supports and expands the efficacy of model validation efforts.

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1. Introduction

Advances in computer hardware technology have allowed the scientific community to build high-resolution computer models capable of simulating complex systems and processes. These computer models can not only evaluate a solution quickly and inexpensively, but also produce dynamic functional output, such as a set of time-series data generated during a process. Since computer simulation technology has quickly advanced, it is critical that the set of verification and validation (V&V) techniques similarly progresses. V&V is an integral part of the simulation development process, one that assesses the accuracy and suitability of the model before relying upon the results.

V&V techniques vary both in quality and applicability to certain models. Often, the quality of the technique may be judged by the amount of subjectivity involved. Basic V&V approaches [1] include subjective, visual comparisons of system data to model data. More advanced methods [2] utilize statistical comparisons of the data that are very complete and more

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objective. The applicability of a particular V&V technique may depend on the nature of the simulation output. For example, simulation output may include discrete forms and functional forms depending on the system being modeled. Discrete simulation output includes measures such as means and variances, while functional output includes time-series data.

It is clear that while there are a wide variety of V&V techniques available, it is important to select an approach that meets both quality and applicability requirements. This paper focuses on objective, statistical validation techniques used to evaluate models that generate functional output. There are several types of validation methods that meet this criteria [3–7]. However, once these validation techniques are applied, if the model is assessed as invalid, analysts are still limited in both knowledge and understanding as to the exact nature of the problem leading to the conclusion of an invalid model. The logical, follow-up question to an assessment of invalidity is, “what is wrong with the model?” If the model generates functional output, such as time-series data, it would be very valuable to identify over what range the model data are a poor representation of the system data. Alternatively, over what range is the model data a good representation of the system? Current techniques stop before answering these resulting questions.

This paper presents a sequential validation methodology that helps answer the resulting questions associated with an invalid model based on functional output. This method first assesses the validity of a model using wavelet analysis of variance (WANOVA). If the model is declared invalid, the wavelet-based test statistic is used in conjunction with a traditional bisection univariate search approach to compare the system and model data and identify the interval with the largest discrepancy. This establishes the region in the signal over which the model data are most biased in relation to the system data. The identification of this biased region in the signal then allows developers to correct the appropriate components of the model.

The paper is organized as follows: Section 2 surveys the available literature on model validation and wavelet-based functional data analysis. Section 3.1 reviews wavelet analysis and WANOVA as a model validation technique. Section 4 presents the WANOVA bisection method for identifying simulation model bias. Section 5 provides a detailed example of the method applied to a simulation study and the results from a large number of simulations. Finally, Section 6 identifies several distinct invalid model scenarios and assesses the performance of the algorithm under these conditions.

2. Literature review

The concept of simulation can be traced back to sampling theory demonstrated with the Buffon Needle Experiment in 1777 in what would become the Monte Carlo simulation method [8]. Since then, the advent of computer technology opened new doors in the field of computer simulation. In 1943, Ulam used one of the first electronic general-purpose computers to conduct computer based simulations that would numerically estimate solutions to intractable problems associated with the Manhattan Project and actually coined the phrase Monte Carlo for the statistical sampling approach [8,9]. With the rise of computer based simulations, some recognized the need to assess the simulation process critically and define a framework of steps to follow to ensure the quality of the resulting simulation. These steps included evaluating the model for both correctness and suitability. In 1979, Sargent [10] presented one of the first in a sequence of papers on simulation validation. Over time, Sargent [10], Balci [1], and Kleijnen [11] developed some of the foundational work on simulation validation. Today, Balci [1] describes verification as “building the model right,” whereas validation evaluates “building the right model.”

Over the years, a wide range of validation techniques have emerged. For example, Balci [2] describes informal techniques that rely on human judgment and dynamic techniques that utilize statistical analysis such as hypothesis testing and confidence intervals. However, one needs to recognize that many established statistical techniques are designed for use with models that generate discrete output. Alternative techniques are required to assess models that generate functional output, such as time-series data. Performing analysis on a single parameter, such as the mean, of the functional data is an oversimplification of the system and model results.

Model validation metrics provide a comprehensive technique for evaluating models that generate time-series data. Validation metrics measure the discrepancy between system and model data by calculating the error associated with different signal components, such as correlation, lag, and magnitude. Together, these errors comprise an overall validation metric that describes the level of agreement between two data signals. Oberkampf and Barone [7] discuss the construction of validation metrics and some recommended features. Several authors including Atkinson et al. [3], Geers [12], Russell [13], and Sarin et al. [14] introduce different versions of validation metrics. However, an important shortcoming with the use of validation metrics is that they still require a subjectively chosen metric value to declare model validity. Accordingly, Sargent [15] expresses concerns with the use of validation metrics and the subjectivity required in their use.

More objective model validation techniques exist within the field of functional data analysis. Functional data analysis is the statistical study of functional data and includes functional analysis of variance (FANOVA). Ramsay and Silverman [16] describe FANOVA as a statistical test on whether a treatment has an effect on the functional response. For time-series data, this basic FANOVA method evaluates a univariate ANOVA for each value of time. Unfortunately, a drawback to this approach is that the dimension of the response can lead to a large number of hypothesis tests and a compounding Type I error rate. Fan and co-workers [5,6,17] have introduced methods to control this Type I error via multivariate statistics and wavelet thresholding. Wavelets may offer benefits in this regard, as they are known for their data compression capabilities.

Wavelets transform data from the time domain to the time-frequency domain. They offer the benefits of smoothing, dimension reduction, and decorrelation of data [18–20]. Several authors [17,21,22] explore wavelet-based functional data analysis, or WANOVA, an approach whose models operate by transforming the data to the wavelet domain and calculating