

Research on Validation Metrics for Multiple Dynamic Response Comparison under Uncertainty

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ABSTRACT

Computer programs and models are playing an increasing role in simulating vehicle crashworthiness, dynamic, and fuel efficiency. To maximize the effectiveness of these models, the validity and predictive capabilities of these models need to be assessed quantitatively. For a successful implementation of Computer Aided Engineering (CAE) models as an integrated part of the current vehicle development process, it is necessary to develop objective validation metric that has the desirable metric properties to quantify the discrepancy between multiple tests and simulation results. However, most of the outputs of dynamic systems are multiple functional responses, such as time history series. This calls for the development of an objective metric that can evaluate the differences of the multiple time histories as well as the key features under uncertainty. In this paper, some researches on investigating validation method and process for dynamic systems with multiple functional outputs are conducted to improve the robustness of existing metrics previously developed by the authors. A vehicle case study is used to demonstrate the comparison study.

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INTRODUCTION

In automobile industry, prototype tests to evaluate the quality and performance of a new vehicle are on the rise. Computer modeling and simulation has become a vital tool in reducing vehicle prototype tests and shortening product development time. To maximize the use of these models, the validity and predictive capabilities of these models need to be assessed objectively and quantitatively. Model validation is the process of comparing CAE model outputs with test measurements in order to assess the validity or predictive capabilities of the CAE model for its intended usage. The fundamental concepts and terminology of model validation have been established mainly by standard committees including the United States Department of Energy (DOE), the American Institute of Aeronautics and Astronautics (AIAA), the Defense Modeling and Simulation Office (DMSO) of the U.S. Department of Defense (DoD) and the American Society of Mechanical Engineers Standards Committee (ASME) on verification and validation of computational solid mechanics, and Computational Fluid Dynamics and Heat Transfer, and various professional societies.

One of the critical tasks is to develop and select a validation metric that has the desirable metric properties for model assessment of a dynamic system with functional responses [1, 2, 3]. One of the key difficulties in model validation for dynamic systems is that most of the responses are functional responses; therefore, the desired objective metric should be able to distinguish the disagreement between test and CAE data throughout the time history and the differences on important features, such as phase shift, magnitude, and slope.

The focus of this paper is to compare the time-history signals or functional responses obtained in all kinds of tests of the passive safety of vehicles and the corresponding numerical simulations, and calculate the level of correlation between multiple non-ambiguous signal pairs. Several quantitative model validation methods have been developed by different researchers in the past ten years [4, 5, 6]. More recently, a few methods were proposed to achieve the validation of computational model with dynamic time history responses [7, 8, 9, 10, 11]. However, these methods emphasize mainly on the whole distribution of the difference between test and CAE curves, but lack of information on major features of the functional responses, such as phase, magnitude, and slope. A metric is regarded as an ideal one if it has most of the desirable characteristics.

such as: objectiveness, generalization, and symmetry. It is also desirable to have physical meaning and can be incorporated with the engineering knowledge. A usable metric, in general, may not possess all these properties. The primary consideration in the selection of an effective metric should be based on the application requirements. Moreover, uncertainty exists in both physical tests and CAE simulations which must be considered during model validation process for dynamic systems. Kennedy and O'Hagan [12] have identified different sources of uncertainty, such as (1) measurement error, systematic error, random errors, and interpolation uncertainty due to lack of samples in the physical tests, and (2) model parameter uncertainty, model inadequacy, numerical or algorithmic uncertainty in CAE simulations.

Depending on whether the uncertainty can be reduced by collecting more information, the above sources of uncertainty have been broadly classified into two categories, aleatory uncertainty and epistemic uncertainty. All of these call for the development of an objective and effective model validation method under uncertainty that can compare the multivariate functional responses of multiple tests and CAE simulations for dynamic systems. What we often face in practical engineering is the validation for multivariate responses, whose features can be mainly stated as the following: (1) multiple response quantities are obtained in a certain condition, which are presented as high dimension data, (2) some responses are highly correlative with each other. Under such condition, when calculating measures of the discrepancies between models and tests using validation metrics, the value of metric of one response may differ from another one. This leads to decision-making problem whether to reject or accept the model when different response quantities offer conflicting inferences. So it is of great importance to address the data correlation and dimension reduction issues before adapting the proposed metric for validation. There are several advanced techniques that can handle this kind of problem, such as principal components analysis (PCA). The PCA is a simple and widely used tool, it considers all samples as a whole and searches for most optimal vectors as projection directions with the criterion of minimize the mean square error. However, the projection directions that are ignored may contain important information as the approach does not consider the characteristics of each response. A novel criterion named Maximum Scatter Criterion (MSC) [13,14] to reduce dimensions with both scatter matrixes between responses and within each response.

Recently, Sprague and Geers, and Knowles and Gear metrics are evaluated [15, 16], but these metrics do not address the correlation of multivariate functional responses. Statistical hypothesis testing is one of the promising approaches to provide quantitative model validation [3, 4]. Bayesian methods have been developed to determine the predictive capabilities of CAE models [4, 5, 6, 7]. They were applied to various model validation problems and showed significant potential. Jiang et al. [6] exploited two advanced statistical techniques for model validation: probabilistic principal component analysis [17] and interval-based Bayesian hypothesis testing. This approach has the potential to address issues such as multiple functional responses, data uncertainty, and response correlation [9,18, 19]. Zhan et al. [20]

proposed an enhanced implementation of the Bayesian method to address the symmetry, mean shift and threshold issues. Liu, et al. [21] summarized four main types of stochastic validation metrics, namely classical hypothesis testing, Bayes factor, frequentist's metric, and area metric, which consider the uncertainty from both physical tests and computer models. However, comprehensive and effective model validation method that considers the uncertainty in both multivariate functional test and CAE data is still rarely found in the literature.

The objective of this research is to investigate and develop model validation methods under uncertainty for dynamic systems with correlated multivariate functional responses. The variability in the tests and CAE data will be considered through distribution based metrics. In the following sections, the proposed new model validation method is first presented, and then a vehicle dynamic system example with multiple functional test and CAE model simulation results is used to demonstrate the effectiveness of the proposed method. Finally, summary is given in the end.

DIMENSION REDUCTION TECHNIQUES FOR MULTIPLE FUNCTIONAL CURVES

When dealing with the multivariate validation, responses with high dimensions and correlations can cause difficulty in making judgment of rejecting or accepting the model intuitively for measures of different responses may offer conflicting inferences. Principal Components Analysis (PCA) is a simple and efficient tool with a broad use. But it regards all the samples as a whole and searches for most optimal vectors as projection directions with the criterion of minimum the mean square error. The projection directions that are ignored may contain important information for the approach does not consider the characteristics of each response. Eigenvalues and corresponding eigenvectors are generated from the covariance matrix of data using a tool called eigenvalue decomposition. Then eigenvalues are regarded as weighting factors for the sake of selecting projection vectors. In the proposed method, the difference between the original normalized CAE and test data is taken as the validation feature. Based on the past experiences, the difference functional data has a much better normality than those of the test or CAE data, which implies that it is more likely to reflect statistical characteristics of a specific distribution (i.e. normal distribution).

Principal Component Analysis (PCA) and Probabilistic PCA

Principal component analysis (PCA) [22] is a well-established statistical method for dimension reduction and has been widely applied to data compression, image processing, exploratory data analysis, pattern recognition, and time series prediction [23]. However, PCA method is not based on a probabilistic model, it cannot handle data uncertainty. Tipping and Bishop [24] proposed a probabilistic principal component analysis method to address this issue. The PPCA is derived from a Gaussian latent variable model which is closely related to statistical factor analysis. The factor analysis is a mathematical technique widely used to reduce the

number of variables (dimension reduction), while identifying the underlying factors that explain the correlations among multiple variables. Details on the application of PPCA method in multivariate model validation should be referred to Ref. [25]. In the Bayesian model validation process, the PPCA approach is exploited and developed to (1) reduce data dimension, (2) address the multivariate correlation, and (3) consider data uncertainty.

For the convenience of formulation, Let $\mathbf{T}$, $\mathbf{C}$ represent the $m \times n$ normalized physical test data and CAE model predictions, where m represents the number of observable variables and n is the corresponding data points. $\mathbf{D}$ represents the difference data between the test and CAE data, i.e., $\mathbf{D}=\mathbf{T}-\mathbf{C}$. The difference data $\mathbf{D}$ is the validating feature selected in this study. The $p \times n$ data matrix Φ represents p principal components and n corresponding data points in the reduced space. Following the PPCA method, the latent variable model relates the correlated data matrix $\mathbf{D}$ to the corresponding uncorrelated latent variable matrix Φ as

$$\mathbf{D} = \mathbf{W}\Phi + \mu_D + \varepsilon \quad (1)$$

where $\mathbf{W}$ is a $m \times p$ weight matrix relating $\mathbf{D}$ and Φ , μ_D consists of m mean values obtained from the difference data matrix $\mathbf{D}$, and ε represents the error or independent noise in $\mathbf{D}$, assuming to be independently distributed Gaussian variables with zero mean and variance $\sigma^2 \mathbf{I}$. The maximum likelihood estimation of σ^2 has a clear interpretation as the variance 'lost' in the PPCA dimension reduction.

With a Gaussian prior over the latent variables defined by $f(\Phi) \sim N(0, \mathbf{I})$, the posterior distribution of the latent variable Φ given the observed $\mathbf{D}$ may be calculated by Bayes' rule as:

$$f(\Phi|\mathbf{D}) \sim N(\mathbf{M}^{-1}\mathbf{W}^T(\mathbf{D}-\mu_D), \sigma^2\mathbf{M}^{-1}) \quad (2)$$

where $\mathbf{M} = \sigma^2 \mathbf{I} + \mathbf{W}^T \mathbf{W}$. This expression represents the reduced difference data with the variability from lost information during PPCA transformation. Let $\Phi^* = \mathbf{M}^{-1}\mathbf{W}^T(\mathbf{D}-\mu_D)$, to test whether the reduced difference data is within an allowable interval, we need to test the distribution of Φ^* while considering the information loss in PPCA transformation. Then the covariance matrix of reduced difference data Σ should include the variance of Φ^* and $\sigma^2 \mathbf{M}^{-1}$. It is calculated as:

$$\Sigma = \Sigma_{\Phi^*} + \sigma^2 \mathbf{M}^{-1} \quad (3)$$

where $\Sigma_{\Phi^*} = \frac{1}{n} \sum_{i=1}^n (\phi_i^* - \mu_{\Phi^*})(\phi_i^* - \mu_{\Phi^*})^T$. The data matrix Φ^* and covariance matrix Σ will be applied in the Bayesian interval hypothesis testing method.

Maximum Scatter Criterion (MSC)

In this study, another technique based on Maximum Scatter Criterion (MSC) [13, 14] is utilized to make the responses independent and reduce dimensions. The concept of Scatter Criterion is popular in the research area of pattern recognition, such as image recognition. In such kind of classifying problem, it aims to project data onto the directions where the scatter of different categories is the maximum for the convenience of classification. As stated before, in the problem of multivariate model validation, the first step is to address the correlations among response quantities and pick up the principal components. The MSC is capable for this goal. By adopting the method, data on the principal projection are with the maximum scatter. While the PCA calculating the eigenvalues and eigenvectors with the covariance matrix, the MSC conduct eigenvalue decomposition based on overall scatter matrix S and scatter within responses S' in Equation 4 and Equation 5.

$$S = (X_i - X_{i_mean})^T (X_j - X_{j_mean}) \quad (4)$$

$$S' = (X_{i_mean} - X_{mean})^T (X_{i_mean} - X_{mean}) \quad (5)$$

With mathematical inference for the scatter matrices, the conclusion we can make is that the overall scatter matrix S is equal to covariance matrix in the PCA. As mentioned before, the projection directions that are ignored by PCA may contain important information. Thus the MSC consider the scatter among responses by subtracting scatter matrix within them from overall scatter. By doing so, more information of the ignored axis would receive more consideration while reaching the goal of reducing dimensions.

It matters a lot to determine the proper number of principal axis after calculating the eigenvalues. When choose the principal components, the intrinsic dimensionality presenting the necessary number of latent variables to contain enough information of original data is utilized. The percentage of the chosen eigenvalues in the whole values quantifies information contained in the principal components.

Let $\mathbf{T} = [t_1, t_2, \dots, t_m]^T$, $\mathbf{C} = [C_1, C_2, \dots, C_m]^T$ denote the real word test data and CAE simulation outputs respectively in dimensionality of $m \times n$. A $p \times n$ ($p < m$) matrix $\Phi_T = [\phi_{T_1}, \phi_{T_2}, \dots, \phi_{T_p}]^T$ represent the p chosen principal components of the test outputs with n points in each response. For the purpose of illustrating, we supposes that the 95% information should be reserved after the propose dimension reduction. Let λ dedicates the quantity of eigenvalue. So the criterion of selecting principal components can be expressed as

$$\sum_{i=1}^p \lambda_i / \sum_{i=1}^m \lambda_i \geq 95\% \quad (6)$$

The corresponding eigenvectors are used to form a $m \times p$ weight matrix $\mathbf{W}$ according to $\lambda_1, \lambda_2, \dots, \lambda_p$.

$$\phi_T = \mathbf{W}^T \mathbf{T}$$

