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Model Predictive Capability Assessment Under Uncertainty

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This paper develops methods to assess the predictive capability of computational models used in system analysis and design. The assumptions and approximations in computational models introduce various types of errors in the code prediction. Although model prediction has error and uncertainty, validation experiments also have measurement errors and variability. Thus model validation involves comparing predictions with test data when both are uncertain. A validation metric based on Bayesian hypothesis testing is presented and the method is extended to consider multiple response quantities or a single model response at different spatial and temporal points. An important need is to extrapolate the validation inference in the tested region to an inference about the predictive capability in the untested region of actual application. A methodology to quantify the confidence in the extrapolation is developed in this paper by propagating inferences across domains using Bayesian networks. The proposed methods are illustrated for application to structural dynamics problems.

Nomenclature

B	=	Bayes factor
C	=	confidence in model prediction
c	=	damping coefficient
D	=	energy dissipated in a lap-joint due to friction
E	=	Young's modulus
F_0	=	amplitude of sinusoidal loading
H_0	=	null hypothesis
H_1	=	alternative hypothesis
h	=	decision variable
k	=	linear stiffness of a component
k_n	=	nonlinear stiffness of a component
n	=	number of data points or realizations
p	=	number of model response quantity variables
$\mathbf{V}$	=	covariance matrix of the experimental data
w	=	uniformly distributed loading
$\mathbf{x}$	=	multivariate model output
z	=	validation data
$\boldsymbol{\alpha}$	=	linking or common variables
$\boldsymbol{\eta}$	=	mean model output vector
$\boldsymbol{\Lambda}$	=	covariance matrix of the model output

I. Introduction

THE advent of modern supercomputers has facilitated increased dependence on numerical models and simulation codes for predicting the behavior of complex engineering systems. However, due to the approximations in the computational models, limited amount of data on the input variables, and physical variability, it is difficult to associate a high degree of confidence with predictions based only on computational methods. The performance of a model may be judged by comparing the outcomes derived from the model against observations made during specific validation experiments. Several sources of physical, statistical and model uncertainties can affect the model prediction, apart from the various sources of error. One way to describe these uncertainties is through probability distributions. When the system properties and load conditions are random variables, the output also becomes a random variable. Similarly, there is uncertainty and error in the experimental measurement of both input data and output response. Thus validation under uncertainty, within a probabilistic context, requires quantification of the model output in terms of a statistical distribution and then effectively comparing it with experimental data that also follow a statistical distribution [1].

Model validation may involve univariate or multivariate comparisons between prediction and observation. A computational model may generate multiple response quantities at a single location or the same response quantity at multiple locations, and a validation experiment might yield corresponding measured responses in a single test. In each case, the multiple responses, being derived from the same input, are correlated. In both cases, model validation involves comparison of multiple quantities of model prediction and test data (multivariate analysis). Bayesian validation metrics are developed and presented in this paper, and illustrated for both univariate and multivariate problems.

One challenge in practical problems is to extend what we can learn about the model's predictive capability within the tested region to an inference about the predictive capability in the application or untested region. Models are often validated in a controlled environment conducting a limited number of small scale tests. Also, the response quantity of interest in the target application may be different from the validated response quantity. In some cases, validation data may be available in the nominal region and the field application may involve off-nominal (tail) behavior. When system-level tests are not feasible, component-level data may be used to make partial inference on the validity of system-level prediction. In all of the above cases, inferences from the validation domain have to be extrapolated to the untested region. Model prediction variance needs to be estimated in the extrapolated region. A Bayesian framework for drawing inferences for predictions in the untested domain is developed and implemented using Bayesian networks (BN) in this paper.

Section II.A proposes several validation metrics using classical and Bayesian hypothesis testing. The metrics compare univariate or

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multivariate model output to the corresponding experimentally observed data and quantify the confidence in the model prediction. In this paper, the validation is formulated using point null hypothesis testing. Bayesian hypothesis testing is able to rationally incorporate various uncertainties to infer how strongly the data supports the null hypothesis as opposed to the alternative hypothesis [2,3]. A quantitative measure of confidence in the model prediction is derived using this approach. In Sec. II.B, Bayes networks are used to extrapolate inferences from the validation domain to the application domain. Because the extrapolation requires uncertainties to be propagated from one variable to the other, the Bayes network appears to be a convenient choice. Thus Bayesian hypothesis testing methodology for validation is extended to extrapolate inferences to the application domain. Two cases of extrapolation are considered in this paper: 1) Extrapolation of validation inferences from one quantity to a different response quantity for which data is absent; 2) the input variables in the validation and application domains are either physically different or different in magnitude. Section III presents several numerical examples to illustrate the implementation of the proposed methods to static and dynamic structural analysis problems.

II. Proposed Methodology

A. Validation Metrics

The fundamental concepts and terminology for the validation of computational codes have been recently established in the literature [4–7]. Currently, the American Society of Mechanical Engineers Standards Committee (ASME PTC#60) on verification and validation in computational solid mechanics has been drafting a set of improved guidelines. Recent work providing procedures in V&V with applications can be found in the literature as well [8–14]. The earlier guidelines on V&V have lacked the incorporation of uncertainty. A validation metric should quantitatively measure the amount of difference between model prediction and experimental data and should also include the uncertainties in them. Whereas our earlier work focused on the inclusion of error estimation in the validation of finite element/difference models and reliability prediction model validation [1,15], this paper proposes an approach for validating models with a univariate and multivariate output, and extrapolates the inferences to the application domains of interest.

Validation is treated as a hypothesis testing problem in this paper. The null hypothesis is that the model is correct and the alterative hypothesis is that the model is not correct. Both classical and Bayesian hypothesis testing methods can be used to derive model validation metrics. This paper focuses on Bayesian methods [15,16] because it is able to link inferences in the validation and application domains. Individual validation is handled with univariate analysis whereas aggregate validation is handled with multivariate statistics. Extrapolation of inferences across various domains is addressed for the first time in this paper incorporating various uncertainties. The proposed Bayesian framework facilitates for conveniently tying validation data to the decision variable to assess the predictive capability of the code in the actual application.

1. Classical Hypothesis Testing

a. Univariate Case. Suppose the model prediction x follows a probability density function $f(x)$ with mean μ_0 and variance σ_0^2. These values are treated as population parameters. The observed data mean and variance of n samples $(y_1, y_2, \ldots, y_n)$ are denoted by $\bar{y}$ and s^2. The model is said to be valid if the sample belongs to the population. A t-test statistic for the mean and F-test statistic for the variance are calculated for the hypotheses.

b. Multivariate Case. Let the multivariate output be represented using a matrix $\boldsymbol{X}$ of size $n \times p$ where n is the number of random realizations and p is the number of different response quantities, or the number of spatial or temporal points at which a single response is predicted or observed. Also $\boldsymbol{\mu}_0$ is the vector of mean values of each column of $\boldsymbol{X}$ and $\boldsymbol{\Sigma}_0$ is their covariance matrix. Let the corresponding observation data matrix be represented as $\boldsymbol{Y}$. Let $\bar{\boldsymbol{Y}}$ be the mean vector and $\boldsymbol{S}$ be the covariance matrix of $\boldsymbol{Y}$. Distance similarity measures based on Mahalanobis distance [13] between the two matrices (observation and prediction) give an idea about how far the centroids of model prediction and data clouds are situated. Similarly, the orientation of the data clouds or the extent of their scatter in each of the principal directions is measured by covariance matrices. Likelihood ratio tests (LRT) [17] are available to test for the covariance similarity between model prediction and data.

It should be noted that in both univariate and multivariate cases, the aforementioned classical statistical tests are only valid under the assumption of normality, that is, x has to be normal and the matrices $\boldsymbol{X}$ and $\boldsymbol{Y}$ have to be jointly normal. When such assumptions are violated, appropriate Gaussian transformations are necessary.

2. Bayesian Hypothesis Testing

Consider two competing models M_0 and M_1 and experimental data D. The Bayes factor [18], defined as $B = P(D|M_0)/P(D|M_1)$ can be used to compare the data support for the two models. If $B > 1$ then the data D favors model M_0 more than M_1. For the sake of validation of a single model, the null and alternative hypotheses may be treated as two competing models as described below.

a. Univariate Case. Let x_0 and x be the predicted response and true response, respectively, of a model M_0. For validation purposes, let us consider the point null hypothesis H_0: $x = x_0$. To estimate the Bayes factor, we need to constitute an alternative hypothesis (H_1: $x \neq x_0$) or model M_1. The probability of observing the data under the null hypothesis $P(\text{data}|H_0\colon x = x_0)$ can be obtained from the likelihood function as $\int \varepsilon f(y|x)g(x)\,\mathrm{d}x$ where $g(x)$ is the prior density of x under the alternative hypothesis. Because no information on $g(x)$ is available, one possibility is to assume $g(x) = f(x)$. The Bayes factor is then computed using the Bayes theorem as

$$B(x_0) = \frac{P(\text{data}|H_0\colon x = x_0)}{P(\text{data}|H_1\colon x \neq x_0)} = \frac{L(x_0)}{\int L(x)g(x)\,\mathrm{d}x} = \frac{f(y|x_0)}{\int f(y|x)f(x)\,\mathrm{d}x} = \left.\frac{f(x|y)}{f(x)}\right|_{x=x_0} \tag{1}$$

Thus, the Bayes factor simply becomes the ratio of posterior to prior PDFs of the predicted response when $g(x) = f(x)$. Further, assuming Gaussian experimental error, we obtain $f(y|x_0) \sim N(x_0, \sigma_{\exp}^2)$ where $\sigma_{\exp}^2$ is the variance of measurement error. Thus measurement uncertainty is explicitly taken into account. The data is said to favor the model if $B(x_0)$ is greater than 1.0. Refer to [1,15] for more a detailed explanation.

Further the confidence in the model prediction, that is, the posterior probability that the null hypothesis is correct, can be estimated as $C = P(H_0|D) = B/(B+1)$. Thus, for example, a Bayes factor of 1.0 would denote 50% confidence in the model prediction implying we do not have enough evidence to reject or accept the null hypothesis.

b. Multivariate Case. Consider p outputs $x = (x_1, x_2, x_3, \ldots, x_p)$ obtained from a computational model; and each model output is treated as a random variable. The joint PDF of the multiple response quantities is denoted by $f_{\boldsymbol{X}}(x_1, x_2, x_3, \ldots, x_p)$. Similarly, experimentally observed response quantities may be treated as a set of correlated random variables $\boldsymbol{y} = (y_1, y_2, y_3, \ldots, y_p)$. Whereas the validation metric for a single response is simply the ratio of its posterior and prior densities evaluated at a particular model prediction value, this univariate case can be extended to a more general multivariate case where the overall metric is defined as the ratio of posterior joint probability density to the prior joint probability density.

For example, if each observation is assumed to have a Gaussian error with constant variance $N(0, \sigma_{\exp}^2)$, then Eq. (1) can be extended to compute the Bayesian validation metric for the multivariate case as

$$B = \frac{\exp[-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{x}_0)^T \boldsymbol{V}^{-1}(\boldsymbol{y} - \boldsymbol{x}_0)]}{\iint \ldots \int \exp[-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{x})^T \boldsymbol{V}^{-1}(\boldsymbol{y} - \boldsymbol{x})] f_{\boldsymbol{X}}(\boldsymbol{x})\,\mathrm{d}x_1\,\mathrm{d}x_2 \ldots \mathrm{d}x_p} \tag{2}$$

The likelihood function for experimental observation was assumed to be proportional to the Gaussian density function. Then a collective comparison can be made using the Bayesian validation metric as shown in Eq. (2) with $\boldsymbol{V}$ being the covariance matrix of the observed data. Again, B is evaluated at a particular model prediction set $(x_1, x_2, x_3, \ldots, x_p)_0$. The data is said to favor the model if B is greater than one. This metric can also be used for a single response quantity predicted at multiple locations of space and time by simply replacing any ith response quantity x_i with $x(t)$. The complicated multiple integration involved in Eq. (2) can be solved using Markov Chain Monte Carlo (MCMC) methods like Gibbs sampling [19].

In the next section, this Bayesian validation methodology is further taken forward to address the issue of extrapolation.

B. Extrapolation Methodology

This section develops a Bayesian methodology to quantify the confidence in model prediction in application domain, based on confidence assessment in the validation domain. Extrapolation is of great importance in various applications and methods have been developed in geographic information science [20], climatic change simulation [21], environmental sciences [22], time series forecasting in finance [23], business management [24], etc. One common practice is to extrapolate the experimental data or confidence bounds to untested domain using trend analysis. However, this approach is of limited use, applicable only when the same response quantity is considered in both validation and application domains, and when there is no change in physics.

A Bayesian methodology is pursued in this section, for two cases of extrapolation. The first case deals with extrapolating validation inferences for one quantity to a different response quantity for which data is absent. The second case addresses the task of validation with change in the input conditions. Further this case can be divided into two categories: 1) A model may be validated using nominal input values for the experimental set up while the decision variable could be the model prediction for tail inputs 2) nature of input condition can be different in validation and target domains, that is, change in type of input loading, material, etc. In both cases, a mathematical link between the target application and validation experiments is established using the Bayes network concept.

1. Case 1: Validated and Decision Variables are Different

Often the quantity validated and the decision variable (quantity of interest in target application) are quite different. Experimental limitations may define the quantity to be measured for the purpose of validating a model. For example, one may validate the axial strain predicted by a model using strain measurements in the laboratory, but the variable that affects the design decision could be shear or torsional stress. Those decision variables can be directly or indirectly related to normal stress through some linking variables. Similarly a decision variable could be the probability of failure of the structure whereas validation may be limited to stress prediction. If the decision variable is not too different from the validated variable, we can accept the model prediction in untested region with some confidence, if a mathematical link between the decision variable and validation domain can be established. When such an explicit relation cannot be established, sensitivity analysis could give a first order relation between the validation and decision variables. The confidence or updated belief in the extrapolation is then derived from the validation metric in the tested region.

Consider a computational model $y(x, \boldsymbol{\alpha})$ in the validated region. Inferences need to be made for a decision variable $h(x, \boldsymbol{\alpha}, \boldsymbol{\beta})$ with $\boldsymbol{\alpha}$ being a set of input random variables (x could represent space or time co-ordinates) and $\boldsymbol{\beta}$ an additional set of random variables in the application domain. Suppose the computational model y is validated using experimental observations z; then the density functions associated with y and hence those of $\boldsymbol{\alpha}$ can be updated using the Bayes theorem. Thus the joint probability distribution and hence the marginal densities of each of the input parameters in $\boldsymbol{\alpha}$ can be updated as

$$f_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}|z) = \frac{f_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) f[z|y(x, \boldsymbol{\alpha})]}{\int f_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) f[z|y(x, \boldsymbol{\alpha})]\,\mathrm{d}\boldsymbol{\alpha}} \tag{3}$$

where $f_{\boldsymbol{\alpha}}(\boldsymbol{\alpha})$ is the prior density, and $f[z|y(x, \boldsymbol{\alpha})]$ is the likelihood function. The updated parameters can then be used to estimate the updated distribution for h by generating input parameters from the posterior density $f_{\alpha}(\boldsymbol{\alpha}|z)$ and substituting them in. The new and old densities of h can then be compared similar to Eq. (1) to assess the predictive capability of the model in the application domain. The ratio, $B_h = f[h(\boldsymbol{\alpha}, \boldsymbol{\beta}|z)]/f[h(\boldsymbol{\alpha}, \boldsymbol{\beta})]$ is treated similar to the Bayes factor in Eq. (1) in assessing the confidence in the decision variable or the model in the application domain. The integration required in Eq. (3) can be calculated using Markov Chain Monte Carlo techniques. The quantities y, z, $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and h can be linked through a Bayes network as shown in Fig. 1.

Bayes networks have been used in artificial intelligence [25], engineering decision strategy [26], safety assessment of software-based systems [27], and model-based adaptive control [28]. Bayes networks have also been applied to the risk assessment of water distribution systems, as an alternative to fault tree analysis [29]. Recently, the Bayes network concept was extended for structural system reliability reassessment [30] by including multiple failure sequences and correlated limit states. Both forward and backward propagation of uncertainty among the components and the system were accomplished. Bayes networks are directed acyclic graphical representations (DAGs) with nodes to represent the random variables and arcs to show the conditional dependencies among the nodes. Each node has a probability density function associated with it. The arc emanates from a parent node to a child node. Each child node thus carries a conditional probability density function, given the value of the parent node. The entire network can be represented using a joint probability density function. The network also facilitates the inclusion of new nodes that represent the observed data and thus the updated densities can be obtained for all the nodes.

The updating methodology is briefly discussed here as follows: Consider the Bayes network U with seven nodes a to g as shown in Fig. 2. Thus $U = \{a, b, \ldots, g\}$. Each node is assigned a probability density function as $f(a)$, $f(b|a)$, $f(c|a)$, $f(d|c)$, $f(e|b, d)$, $f(f)$ and $f(g|e, f)$. In the context of this paper, the variables or nodes a, b, etc., may correspond to input random variables as well as quantities computed at each step of the computational process. The joint PDF of the entire network is the product of PDFs of various nodes in the network, that is,

$$f(U) = f(a) \times f(b|a) \times f(c|a) \times f(d|c) \times f(e|b, d) \times f(f) \times f(g|e, f) \tag{4}$$

Note that for nodes b, c, d, e, and g, only the conditional densities are defined and included in the joint PDF in Eq. (4). The marginal PDF of b (for example) can be obtained by the integration of the joint PDF over all the values of the remaining variables. This integration is conveniently done using Markov Chain Monte Carlo techniques [19].

The joint probability density function for the network can be updated using the Bayes theorem when data is available. Assume that some evidence or test data m for node b is available. A new node m is now added to the network (see Fig. 3); this new node is associated with a conditional density function $f(m|b)$. Then the joint PDF

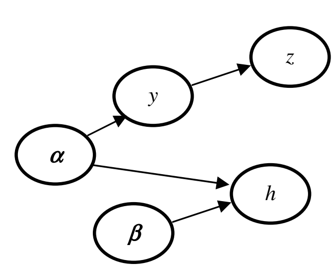


Fig. 1 Bayesian network representation of validation and extrapolation.

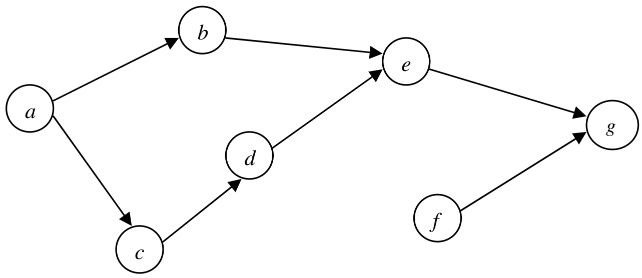


Fig. 2 Bayes network before data is collected.

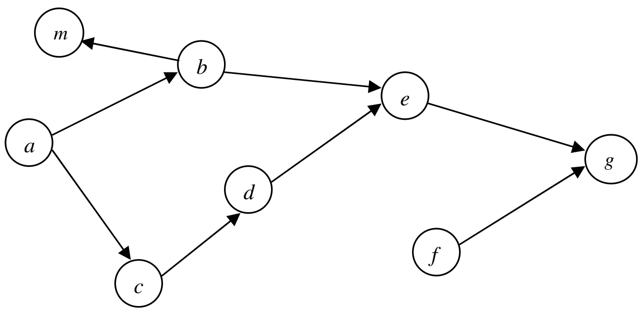


Fig. 3 Updated Bayes network with additional data node.

$f(U, m)$ for this new network is

$$f(U, m) = f(a) \times f(b|a) \times f(c|a) \times f(d|c) \times f(e|b, d) \times f(f) \times f(g|e, f) \times f(m|b) \quad (5)$$

With this new joint density, the posterior marginal densities of each of the nodes can be estimated by integrating the joint density over the range of values of all other nodes. Thus the node b represents the validated variable whereas node g represents the decision variable.

2. *Case 2: Extrapolation for Changes in Input Conditions*

Sometimes the variable in the validation domain could be the model prediction y evaluated at the nominal value of input variable whereas the decision variable h could be the prediction made using the same model for the input from the tail region, or vice versa. For instance, in reliability analysis, failure may occur in the tail regions of the distributions of the input random variables, but experimental data may be available only at nominal values. Thus B_y could be $f(y|z)/f(y)$ evaluated at $\boldsymbol{\mu}_{\boldsymbol{\alpha}}$ whereas B_h could be the ratio $f(y|z)/f(y)$ evaluated at $(\mu + 2\sigma)_\alpha$.

The Bayes network shown in Fig. 1 applies to this case as well. Now, h is basically the same variable as y; the distinction is that h is evaluated at the tail of the input probability density function and y is evaluated at nominal values of the input. Thus this is a special case of the general extrapolation in case 1 where y and h could be physically different quantities.

Sometimes, the input variables in the validation and application domains could be completely different although the model response variable is the same quantity. For example, input conditions like type of loading (i.e., distributed vs concentrated load), material properties (e.g., linear vs nonlinear elasticity), geometry and boundary conditions (e.g., rigid vs flexible joints) could be physically different. In all these cases, we need linking variables that connect the two domains.

Another case of extrapolation is system-level model assessment when only component-level data is available. This has been addressed by the authors in an earlier paper [16]. A large system of codes can be decomposed into subsystems, components, etc., and represented using a Bayesian network. Once data is available on any of the component-level nodes, then all nodes, including system-level nodes can be updated. The posterior and prior distributions of the system-level nodes can give an estimate of confidence in the code prediction of system-level quantities.

Thus the Bayes network approach offers a rational and effective methodology to extrapolate inferences from the validation domain to the application domain, as long as the two domains have common, linking nodes.

III. Numerical Examples

Several numerical examples illustrating Bayesian validation and extrapolation methodologies are discussed in this section. The examples, however, are limited to a few cases only to maintain the brevity of the paper.

A. Example 1: Validation of a Three-Parameter Energy Dissipation Model for Lap Joints

Here we consider a three-parameter model [11] to predict the dissipation energy D released per cycle at the joint when subjected to impact harmonic force amplitude of F_0. The energy loss in the joint under one cycle of sinusoidal loading is found by integrating the area under the hysteresis curve and analytically derived as

$$D = k_n \left(\frac{n_1 - 1}{n_1 + 1} \right) \Delta z^{n_1 + 1} \quad (6)$$

where k_n is a nonlinear stiffness, n_1 is a nonlinear exponent, and Δz is the displacement amplitude obtained by solving the equation:

$$2F_0 = k\Delta z - k_n \Delta z^{n_1} \quad (7)$$

where k is a linear stiffness term. The three parameters n_1, k_n [or $\log_{10}(k_n)$ in this case] and k are quantified from the experiments and the statistics are given in Tables 1 and 2. Each of these parameters is found to follow a normal distribution.

Validation experiments were conducted at Sandia National Laboratories [11] at five levels of loading, that is, 60, 120, 180, 240, and 320 lb that span the range of loadings the system may be exposed to. The same five levels are used in the model computation. Twelve sets of experimental data were obtained by dismantling the structure and reassembling it, thus simulating the stochasticity in structural assembly. The mean values of energy predicted (×) at different load levels are plotted against the data (−) in Fig. 4.

The data obtained through the Sandia experiments are used in this paper to make individual comparisons (at each of the five different loadings) as well as collective comparisons, using Bayesian hypothesis testing. See the Appendix for actual test values. The mean values of energy at different load levels (five in this case) are assumed to be random variables that are being updated using the available test data. The posterior and prior densities of those means can be used to calculate the marginal Bayes factors as shown in Eq. (1) or the collective metric as given by Eq. (2), assuming Gaussian experimental error. Table 3 shows the priors and posteriors obtained using a Markov Chain Monte Carlo procedure. All the energy values are transformed to logarithmic scale for the sake of simplicity in Table 3 and Bayes factor computation and hence the validation is

Table 1 Statistics of parameters

Variable	n_1	$\log_{10}(k_n)$	k
Mean	1.36	5.855	1,172,700
Std. dev	0.068	0.1866	12,865

Table 2 Correlation coefficients among model parameters

n_1	$\log_{10}(k_n)$	k
1	0.902	0.494
0.902	1	0.2295
0.494	0.2295	1

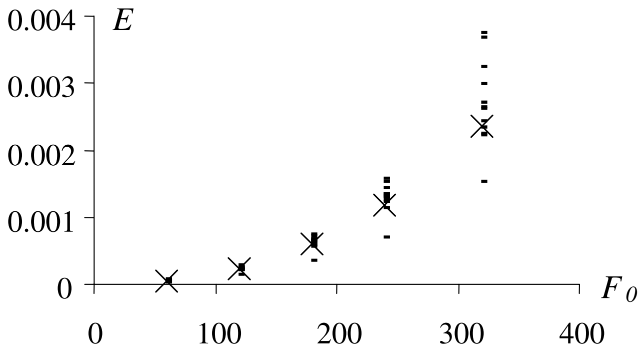


Fig. 4 Force amplitude vs energy.

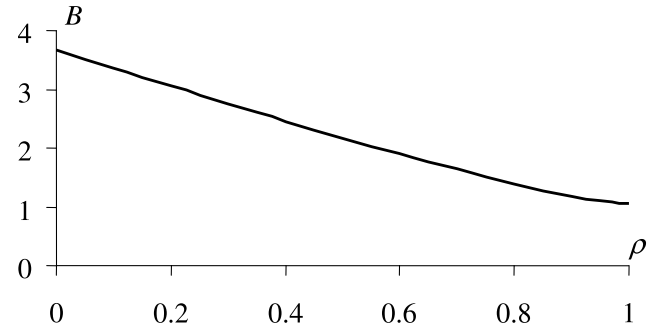


Fig. 5 Effect of correlation among model outputs on validation metric.

carried out in original space only. Table 3 shows that the data gives about 50% confidence (i.e., $B \approx 1$) in the model at all five load levels. The aggregate Bayes factor as per Eq. (2) is also found to be **1.06** indicating about 50% confidence in the model overall.

In multivariate model validation, the model assessment metric can be affected by the correlation structure among the multiple response quantities of interest. Suppose the multivariate model prediction $\boldsymbol{x}$ is normal with mean vector $\boldsymbol{\eta}$ and covariance matrix $\boldsymbol{\Lambda}$. Having observed the data $\boldsymbol{y}$ with Gaussian measurement uncertainty (multivariate normal likelihood) having zero mean and covariance structure $\boldsymbol{V} = \mathrm{cov}(\boldsymbol{y})$, the posterior joint density for $\boldsymbol{x}$ will be multivariate normal as well. The posterior mean vector and covariance matrix for the model output are given by

$$\boldsymbol{\eta}_p = (\boldsymbol{\Lambda}^{-1} + \boldsymbol{V}^{-1})^{-1}[\boldsymbol{\Lambda}^{-1}\boldsymbol{\eta} + \boldsymbol{V}^{-1}\bar{\boldsymbol{y}}], \qquad \boldsymbol{\Lambda}_p = (\boldsymbol{\Lambda}^{-1} + \boldsymbol{V}^{-1})^{-1} \tag{8}$$

The aggregate validation metric is computed at the mean value $\boldsymbol{\eta}$ as

$$B_y = \left.\frac{f(x|\boldsymbol{y})}{f(x)}\right|_{\boldsymbol{\eta}} = \frac{|\boldsymbol{\Lambda}|^{1/2}}{|\boldsymbol{\Lambda}_p|^{1/2}} \exp[-\tfrac{1}{2}(\boldsymbol{\eta} - \boldsymbol{\eta}_p)^T \boldsymbol{\Lambda}_p^{-1}(\boldsymbol{\eta} - \boldsymbol{\eta}_p)] \tag{9}$$

Suppose we need to assess the confidence in an arbitrary model output at $\boldsymbol{x}$, the Bayes factor is calculated as

$$B_h = \left.\frac{f(x|\boldsymbol{y})}{f(x)}\right|_{\boldsymbol{x}} = \frac{|\boldsymbol{\Lambda}|^{1/2}}{|\boldsymbol{\Lambda}_p|^{1/2}} \frac{\exp[-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\eta}_p)^T \boldsymbol{\Lambda}_p^{-1}(\boldsymbol{x} - \boldsymbol{\eta}_p)]}{\exp[-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\eta})^T \boldsymbol{\Lambda}^{-1}(\boldsymbol{x} - \boldsymbol{\eta})]} \tag{10}$$

Thus the decision variable $\boldsymbol{x}$ can be prediction obtained for tail input values. It is clear from Eqs. (9) and (10) that the Bayes validation metric depends on the correlation structure among model output variables and the corresponding experimentally observed quantities. In this example, all the elements of the correlation matrix (size 5×5) for the model output are close to 0.98.

For the sake of illustration, consider a simple case where the off-diagonal elements of the correlation matrix ρ_{ij} $(i \neq j)$ are all equal to ρ. For values of ρ ranging from 0–1, the relation between the Bayes factor B and ρ can be plotted as in Fig. 5, using Eq. (9). (Obviously, all ρ_{ij}'s will not have the same value; this is to simplify the plot to two dimensions).

When the correlations among the multivariate model output are ignored, the overall Bayes factor is found to be 3.67 and it is also the product of the individual Bayes factors (i.e., 1.21, 1.07, 1.34, 1.38, 1.25) for the predictions at each of the five load levels. These marginal B values are slightly different from those computed for the original model output with correlations, as given in Table 3. Thus the Bayes factor metric (individual or overall) properly accounts for the correlation structure among various model outputs.

Table 3 Bayes factors for energy dissipation model: individual comparisons

	Prior		Posterior		B
F_0 lb	μ_μ	σ_μ	μ_μ	σ_μ	$f(\mu_\mu)/f(\mu_\mu)\vert\mu_\mu$
60	4.362	5.537	4.358	5.564	1.053
120	3.645	4.968	3.643	4.996	1.063
180	3.224	4.54	3.221	4.571	1.061
240	2.925	4.192	2.922	4.217	1.05
320	2.626	3.735	2.622	3.765	1.063

B. Example 2: Extrapolation of Stress Prediction from Nominal to Tail Loading

A mechanical component in an application is a square plate structure with a circular hole in the center. The plate is subjected to distributed loading along the two straight edges. Finite element (FE) modeling may be used to predict any response quantity of interest related to this plate. The FE model of a quarter the structure is used due to the symmetry, as shown in Fig. 6, and the vertical displacement of tip A under the loading is of interest.

The plate has dimensions of $24 \times 24 \times 1$ in.^{3} and the curved edge has a radius of 8 in. The Young's modulus E and the Poisson ratio is v are Gaussian random variables with statistics N (10,000; 2000) psi and N (0.2, 0.025), respectively. The plate is subjected to uniform loading of equal magnitudes along its edges. For the purpose of analysis, the loading on each edge is assumed Gaussian with statistics $w \sim N$ (500, 50) kips. Elastic small deflection theory was used in the analysis to determine the displacement of tip A. Appropriate boundary conditions were applied along the other straight edge portions of the plate.

Because the input loading and material properties are random, the model response is also a random quantity. One can estimate the statistical distribution of model response by running the FE code several times using randomly sampled values of the input loading (w, E, v) each time. To avoid this computationally intensive exercise, a stochastic response surface [31] using polynomial chaos expansion [32] was used in this example to represent the tip displacement as a function of the distributed loads along the edges. Although we considered the Poisson's ratio v as a random variable, analysis of variance showed that v has insignificant contribution to the variance of y and hence v is omitted in the response surface. Thus the model output is a function of E and w. To fit a second order response surface as given in Eq. (11), nine actual finite element evaluations were required.

The stochastic response surface with $R^2 = 0.999$ is

$$y = 1.5306 - 0.3326\xi_1 + 0.1544\xi_2 + 0.0666(\xi_1^2 - 1) - 0.03329\xi_1\xi_2 \tag{11}$$

where ξ_1 and ξ_2 are independent standard normal variables. Here ξ_1 and ξ_2 are related to the physical variables E and w using the relation $E = 10,000 + 2000\xi_1$ and $w = 500 + 50\xi_2$. Thus the model response (vertical displacement at tip A) for any values of E and w can be obtained by first transforming each of those values into standard normal space and then substituting them in Eq. (11). Refer to [28,29] for more details on stochastic response surface methods.

Suppose we validate this model in a test setup at its mean input values ($w = 500$, $E = 10,000$) whereas in the actual application, the plate experiences larger loads ($w = 750$, $E = 10,000$).

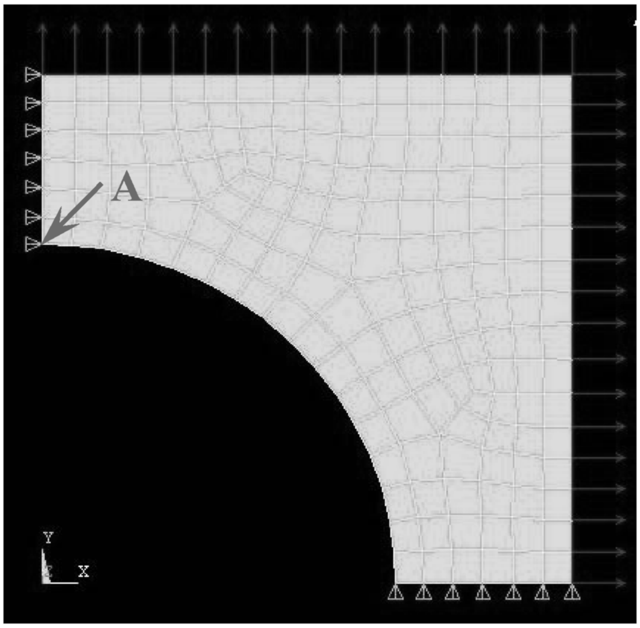


Fig. 6 FE model of the plate.

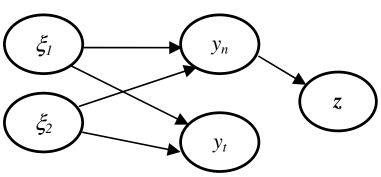


Fig. 7 Bayes network for the plate problem: Nominal input to tail input.

This is case 2 in Sec. II.B.2, where the validation and decision variables are identical but evaluated at mean and tail loads, respectively. The test data z is given in the Appendix. The Bayesian network depicting the relations between various quantities is given in Fig. 7. Both y_n (nominal) and y_t (tail) are exactly the same functions of ξ_1 and ξ_2 but the response values are evaluated at different inputs. The validation metric B_{yn} at the mean input value is found to be 1.52, which corresponds to 60.3% confidence [i.e., $B_{yn}/(B_{yn}+1)$]. The confidence in the model prediction for any other input value (say, from its tail region) can be calculated, as explained in Sec. II.B.2, by evaluating $B_{yt} = f(y|z)/f(y)$ at this new input value (from the tail region) first and then by computing C_h using the relation $C_h = B_h/(B_h+1)$. Given the experimental data at nominal loading, the confidence in the model prediction at different load values (equal magnitude on all edges) is estimated and shown in Fig. 8. At $w = 750$, $B_h = 0.142$, and $C = 12.46\%$. As we collect more data at higher load values, one should expect the confidence curve to move to the right, indicating increasing confidence at higher loads. With the current information, the confidence drops below 50% at $w = 612$ lb. Thus the proposed methodology can also be used to determine the limits of extrapolation.

C. Example 3: Different Loading Conditions

For the problem in example 2, suppose the plate is subject to uniform loading w of equal magnitude along its edges in the validation domain and point load P in the application domain. It is assumed that the load P acts at the midpoint along the edge of the quarter plate. For the purpose of analysis, the loading on each edge is assumed Gaussian with statistics $w \sim N$ (500, 50) kips and $P \sim N$ (6000, 1200) kips. Further the material properties are random variables as well with distributions $E \sim N$ (10,000; 1000) psi while $v \sim N$ (0.2, 0.025). A linear elastic, small deflection theory was used in the analysis to determine the displacement of tip A shown in Fig. 4. Because the input loading is random, the model response in both

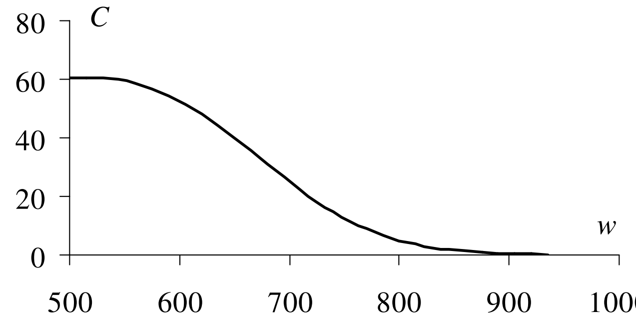


Fig. 8 Confidence in prediction at non-nominal loads.

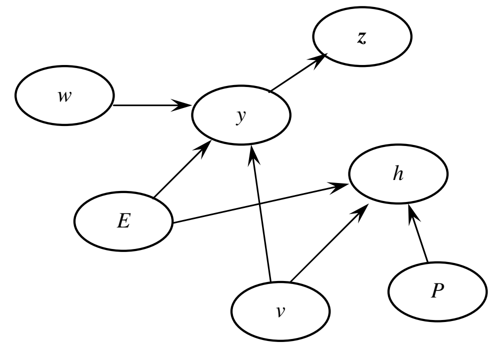


Fig. 9 Bayes network for the plate problem: different loading conditions.

domains will also be a random quantity. The FE model is the only common link between the two domains. The BN for this problem is shown in Fig. 9 and the common independent variables are E and v.

Model y represents the response under distributed loading whereas h represents response under point loading. The stochastic response surface is constructed for h in terms of E and P only because the variable v is found out to have no significant effect on h.

The stochastic response surface with $R^2 = 0.999$ is

$$h = 0.5623 - 0.1222\xi_1 + 0.1134\xi_3 + 0.02447(\xi_1^2 - 1) - 0.02445\xi_1\xi_3 \tag{12}$$

where ξ_1 and ξ_3 are standard normal variables related to E and P using the relations $10,000 + 2000\xi_1$ and $6000 + 1200\xi_3$, respectively. Suppose the data z from example 2 (as given in the Appendix) is used to update the response in the validation domain y, then the linking variable E and hence the decision variable h are updated through the Bayes network. The Bayes factors for y and h evaluated at the mean values of E, w, and P are estimated to be 1.52 and 1.1, respectively. This is case 2 in Sec. II.B.2 where the input conditions are physically different in the validation and extrapolation domains.

D. Example 4: Validation and Extrapolation for a Spring-Mass System

The safety of critical aerospace components is dependent on their structural connections with the surrounding support structure. Analytical models can be developed to predict the component response to sinusoidal environmental loadings. The response quantity of interest in both the validation and application domains is the maximum acceleration experienced by a mass supported by these joints. Suppose the validation domain involves a single spring tested under a sinusoidal loading while the application domain, a three-legged system supporting a mass subject to sinusoidal as well as arbitrary loading.

For simplicity, let the joints be modeled using springs with k and c. The mass attached on the top of the joint is $m = 5$. For a three-legged system, the individual bolts (or springs) are assumed to have identical properties and hence same statistics. The maximum amplitude of the force at any time for a given type of loading is limited to 100 lb. The sinusoidal excitation at the base has a frequency of Ω rad/s. The experimental error in measuring the acceleration of the mass is assumed to be Gaussian with zero mean and variance of 9 in/sec^2. For the three-legged system, each spring is assumed to be inclined making an angle θ_i for $i = 1, 2, 3$, to the horizontal. This angle is assumed to be random to model the uncertainties in the configuration of the connections and errors made in their assembly.

The statistics of various parameters are shown in Table 4. Figure 10 shows the simplified models of the structural joints. All the numerical values used in this particular example are chosen only for the sake of illustration.

The maximum acceleration transmitted to the mass for a sinusoidal loading is given for the single leg model as [33]

$$\ddot{y}_{\max} = \frac{F_0}{m}\frac{\sqrt{1 + (2r\zeta)^2}}{\sqrt{(1 - r^2)^2 + (2r\zeta)^2}} \tag{13}$$

where the frequency ratio $r = \Omega/w$, natural frequency $w = \sqrt{k/m}$, and damping factor $\zeta = c/2mw$. For the three-legged system, the effective stiffness and damping coefficient are estimated as

$$k = \sum_{i=1}^{3} k_i \sin\theta_i$$

and

$$c = \sum_{i=1}^{3} c_i \sin\theta_i$$

respectively, and substituted in Eq. (13) to predict the acceleration of the mass. The statistics of k_i and c_i in each leg of the three-legged system are the same as for the single leg system (Table 4) to indicate that the same type of joints are used in the 3-legged system; however, there is variability from joint to joint.

The various validation and extrapolation activities to be conducted as part of this example are summarized in Table 5. The observed acceleration values on the single leg are given in the Appendix. The quantity of interest is maximum acceleration in all examples. Three cases of extrapolation are considered in this example. In case 1, the response of a single spring is validated under sinusoidal loading and inferences need to be extrapolated to the acceleration under arbitrary loading for the same single leg structure. In case 2, the application domain involves a three-legged system subject to sinusoidal loading. This can be treated as a system-level model assessment. Case 3 deals with system-level model assessment and change in input conditions at the same time.

Thus the different cases of extrapolation discussed in Sec. II.B are simultaneously considered in this example. The response quantity (maximum acceleration) for arbitrary loading requires that the loading be expressed as a Fourier series of sines and cosines. Then Eq. (13) is repeatedly used for several Fourier components of the load and the summation of all such individual responses is used to calculate the decision variable.

In this example, triangular and parabolic pulse loads are used in the application domain and load types are shown in Fig. 11. The results obtained in each case are summarized in Table 6. The variable B refers to the validation metric in the each domain. The ratio B, defined in Eq. (1), is always evaluated the mean value of the model prediction in this example.

A Bayes factor for the decision variable close to 1.0 indicates that validation data are not informative for assessing the model in the application domain. In general, the value of B in the extrapolation domain is lower than in the validation, as expected, because there should be less confidence in the extrapolation than in the domain where data is available.

The numerical examples in this section illustrated the proposed methodology for model validation and then extrapolation. Example 1 demonstrated the use of validation metrics for marginal and collective comparisons. The problem was limited to multivariate Gaussian outputs but it can be extended to more general cases. When there are no closed-form expressions available for generalized multivariate density functions in Eq. (2), appropriate transformations will be needed to compute them numerically.

The Bayesian network methodology for extrapolation in examples 2 and 3 required the statistical distribution of the computational model output. For some practical problems involving highly nonlinear models and with a large number of input variables, the response surfaces as given in Eqs. (11) and (12) can be approximate. In this paper, the length of the Markov Chain was set at 50,000 runs to achieve sufficient convergence. However, the number of actual response surface or model evaluations may be much higher than the length of the chain due to the rejection sampling nature of MCMC simulation. Methods to reduce the number of function evaluations within MCMC are currently being explored. Also, in some situations, the explicit relationships or linking variables may not be available for application and validation domain. Sensitivity analysis can be used to establish at least first order relations among different variables.

IV. Conclusion

This paper addressed the validation of computational models by comparing model outputs against observations from the experiments. Both univariate (individual) and multivariate (aggregate) comparisons can be implemented using hypothesis tests. In this paper, Bayesian statistics were used to derive the required validation metrics. The Bayesian methodology helps to propagate inferences from the validation domain to the target application domain through the Bayes network approach. Two cases of extrapolation were considered: extrapolation of validation inferences from one response quantity (for which data is available) to a different response quantity (for which data is absent), and from one input condition to another. The second case included two situations: the input variables in

Table 4 Statistics of parameters in the spring-mass system

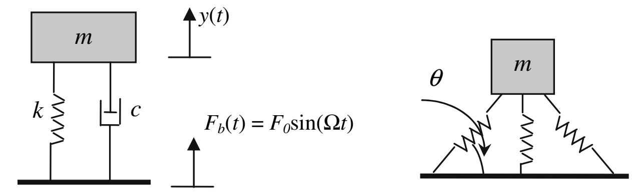
Parameter	Type	Mean	Std. dev
k	Lognormal	1000	100
c	Lognormal	7	2
Ω	Normal	5	1
θ	Normal	45 deg	5 deg

Table 6 Summary of validation and extrapolation results for the four cases

Case	B in validation domain	B in application domain
1	1.82	1.04 (parabolic pulse) 1.03 (triangular pulse)
2	1.82	1.62
3	1.82	1.1 (parabolic pulse) 1.1 (triangular pulse)

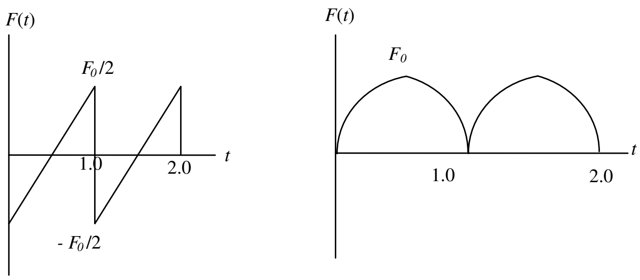
Table 5 System-level model assessment activities

Case	Validation domain	Application domain	Response quantity	Loading in validation domain	Loading in application domain
1	Single leg	Single leg	Acceleration	Sinusoidal	Arbitrary
2	Single leg	3-Legged	Acceleration	Sinusoidal	Sinusoidal
3	Single leg	3-Legged	Acceleration	Sinusoidal	Arbitrary



a) Single leg b) Three-legged system

Fig. 10 Spring-mass system.



a) Triangular load b) Parabolic load

Fig. 11 Pulse loading.

validation and application domains are physically different, and the inputs in the two domains come from two regions of a distribution.

The marginal validation metrics are derived from posterior and prior densities of model outputs. Also the probability density of the decision variable (in the application domain) is updated indirectly using data in the validation domain. Both tasks are achieved and combined effectively by Bayesian computations. The methodologies are demonstrated using numerical examples with closed-form expressions for model output. The techniques can be extended to more practical problems. If the system analysis model is a large finite element code, the computational effort in Markov Chain Monte Carlo simulations for Bayesian updating is expensive. In that case, a response surface approximation might be useful, as shown in one of the numerical examples.

The Bayesian network approach for extrapolation works only in the context of Bayesian validation metrics such as Bayes factor. If classical statistics-based metrics are used for model validation, the extrapolation methodology still needs to be developed. This paper addressed model validation from a hypothesis testing perspective. Validation can also be approached from a decision-making perspective, facilitating trade-off between cost of wrong prediction vs cost of additional information for model refinement. Quantitative methods for such an approach need to be investigated, considering various uncertainties.

Appendix

The experimental data used in various numerical examples are provided in this section.

Example 1

Twelve replicates of experimental results (observed energy values) are given in Table A1.

Example 2

The displacement data (five samples) corresponding to the mean load input are $z = \{1.215, 1.563, 1.618, 1.962, 1.294\}$.

Example 3

The data used in the example are the same as those used in example 2.

Table A1 Twelve replicates of experimental results (observed energy values)

$F_0 = 60$ lb	$F_0 = 120$ lb	$F_0 = 180$ lb	$F_0 = 240$ lb	$F_0 = 320$ lb
5.983E-05	0.000262	0.000645	0.001290	0.002974
6.585E-05	0.000278	0.000748	0.001576	0.003679
5.344E-05	0.000223	0.000631	0.001520	0.003748
5.403E-05	0.000216	0.000586	0.001342	0.003234
4.012E-05	0.000208	0.000545	0.001128	0.002330
4.103E-05	0.000208	0.000576	0.001223	0.002637
4.632E-05	0.000223	0.000629	0.001346	0.002697
2.963E-05	0.000128	0.000354	0.000696	0.001517
4.121E-05	0.000228	0.000660	0.001247	0.002220
3.937E-05	0.000218	0.000661	0.001323	0.002618
4.701E-05	0.000257	0.000718	0.001423	0.002422
4.172E-05	0.000224	0.000636	0.001287	0.002251

Example 4

All cases used 12 values of observed accelerations as $z = \{21.639, 22.940, 24.940, 21.696, 24.816, 25.704, 23.163, 22.250, 20.816, 23.354, 22.813, 23.661\}$

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