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An exercise in model validation: Comparing univariate statistics and Monte Carlo-based multivariate statistics

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ABSTRACT

The complexity of mathematical models used by practicing engineers is increasing due to the growing availability of sophisticated mathematical modeling tools and ever-improving computational power. For this reason, the need to define a well-structured process for validating these models against experimental results has become a pressing issue in the engineering community. This validation process is partially characterized by the uncertainties associated with the modeling effort as well as the experimental results. The net impact of the uncertainties on the validation effort is assessed through the "noise level of the validation procedure", which can be defined as an estimate of the 95% confidence uncertainty bounds for the comparison error between actual experimental results and model-based predictions of the same quantities of interest. Although general descriptions associated with the construction of the noise level using multivariate statistics exists in the literature, a detailed procedure outlining how to account for the systematic and random uncertainties is not available. In this paper, the methodology used to derive the covariance matrix associated with the multivariate normal *pdf* based on random and systematic uncertainties is examined, and a procedure used to estimate this covariance matrix using Monte Carlo analysis is presented. The covariance matrices are then used to construct approximate 95% confidence constant probability contours associated with comparison error results for a practical example. In addition, the example is used to show the drawbacks of using a first-order sensitivity analysis when nonlinear local sensitivity coefficients exist. Finally, the example is used to show the connection between the noise level of the validation exercise calculated using multivariate and univariate statistics.

1. Introduction

While dealing with the issues involved in full-scale V&V exercises, the reason for simulation in the first place is easily forgotten. The purpose of a model is to simulate real world physical processes which govern the quantities being studied in hopes that insight will be gained regarding the behavior of such quantities. If experimental results existed or were easily obtained for every possible situation, there would be no need for these simulations. Moreover, many times, experimentation is not feasible at the highest level due to lack of funds, security reasons, or simply due to lack of complete understanding of the physics involved. However, the ability to predict physical processes approaching the level of complexity of the quantity of interest builds confidence in a model's ability to make predictions at the highest level of interest. Obviously, the ability of a model to make predictions at the highest level depends heavily on the complexity of the model (i.e. what are the modeling assumptions). The author's experience has shown that many models being used in engineering are located at opposite ends of the modeling spectrum from simple to complex models. These two types are as follows:

(1) *Simple models based on many simplifying assumptions used to simulate very specific cases*. These models are useful in studying slight variations of some relatively specific quantity of interest. However, they may not be reliable in predicting quantities outside the specific case or set of assumptions.
(2) *Extremely complex models used to fully model complex physical phenomena*. This type of model is usually computationally expensive but may be used to study a wide variety of quantities of interest with some level of confidence.

As computational power increases, so does the ability to fully resolve the complex physical phenomena associated with quantities of interest at the highest level (Type 2 models).

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Our increasing ability to model real world quantities at the highest level of complexity may decrease the need for experimental data to validate these quantities in the future. However, Type 1 models are still prevalent in the engineering community.

As stated earlier, Type 1 models are used to examine specific cases under simplifying assumptions. Often times, these simplifying assumptions greatly affect the uncertainty estimates associated with the model inputs or experimentally measured variables. For example, it is common to assume constant fluid properties when a temperature dependence is needed. This simplifying assumption results in the need for a larger uncertainty estimate associated with the fluid properties. In some instances, this increases the possibility of nonlinear local sensitivity coefficients within the model input uncertainty bands. In many cases, the output(s) of interest (i.e. experimental/ simulation/ comparison error results) may be assumed to follow a univariate/ multivariate normal distribution based on the Central Limit Theorem. In these cases, the noise level of multiple realizations of the outputs of interest may be described by the multivariate normal probability density function (*pdf*). However, this distribution may not be correctly defined using the traditional linear propagation of errors approach because of nonlinear local sensitivities. In these cases, sampling methodologies such as Monte Carlo analysis are useful. Clearly there is a desperate need for standardized validation procedures which can be used in these situations. There exist several quantitative validation metrics in the literature that provide methodologies to estimate the error associated with modeling assumptions provided that benchmark experimental data exists at similar conditions to the reality of interest being modeled [1–3]. In the following paper, an end-to-end validation example using a multivariate first-order sensitivity analysis and Monte Carlo analysis is performed and discussed using both univariate and multivariate statistics. This example examines the validity of a single-zone combustion model used to simulate the electrical output of a natural gas internal combustion engine/generator set. This is a key example of a Type 1 model commonly used to predict different quantities of interest for a specific case and set of simplifying assumptions [4–7].

2. Experimental setup

Of course, experimental data lays the foundation upon which we can begin to build a V&V exercise. A schematic of the experimental apparatus is presented as Fig. 1. The engine/ generator set is a 1.5 L natural gas internal combustion engine connected to a 15 kW generator. This engine/generator set was modified in order to recover waste heat from the coolant jacket and exhaust gases. Modifications include: removal of the thermostat used to control the coolant flow, replacement of the conventional belt-driven radiator fan with an electric fan, and the addition of instrumentation which is described later in this paper.

The engine was operated at a constant speed in order to follow an electrical load; therefore, the fuel input was constantly throttled to meet these requirements. The engine specifications are presented as Table 1.

Each instrument used in the experimentation was either calibrated by the manufacturer or in-house. Calibration sheets were provided for cases where calibrations were made by the manufacturer of the instrument. The natural gas flowmeter is a Flocat LA10 laminar flow element device which uses the pressure and viscosity of the natural gas in the laminar region to produce a linear 4–20 mA output. All flowmeters were calibrated by the manufacturer over a prescribed range similar to the design test conditions. The total power produced by the generator was measured using a transducer capable of measuring up to 100,000 W.

3. Experimental procedure and results

The objective of this experiment was to vary the natural gas flowrate on the engine/generator set in order to monitor the power output. This procedure was accomplished by simply incrementing the load on the generator from approximately 2–11 kW using the 0–15 kW power transducer to monitor the process. The experimental results for the total electrical power output are presented in Fig. 2. Fig. 2 shows that in order to vary the electrical output of the generator from approximately 2–11 kW, the fuel flowrate was varied from approximately 1.0–2.7 ft^3/min.

4. Experimental uncertainty analysis

The uncertainty analysis presented in this section was conducted according to the American Society of Mechanical Engineers Performance Test Code 19.1 [8]. Using this methodology, the standard uncertainty is equivalent to half the uncertainty as presented in Coleman and Steele [9] at the 95% confidence level. The standard uncertainty in a result is shown using the

Table 1
Engine characteristics.

Type	In-line OHV, SOHC
Number of cylinders	4
Combustion chamber	Semi spherical type
Total displacement	1468 cm^3
Cylinder bore	75.5 mm
Piston stroke	82.0 mm
Connecting rod length	131 mm
Compression ratio	9.0
Speed	1800 RPM
Valve timing	
Intake opening	BTDC 14°
Intake closing	ABDC 48°
Exhaust opening	BBDC 55°
Exhaust closing	ATDC 13°
Fuel injection	BTDC 35°
Exhaust closing	ATDC 13°

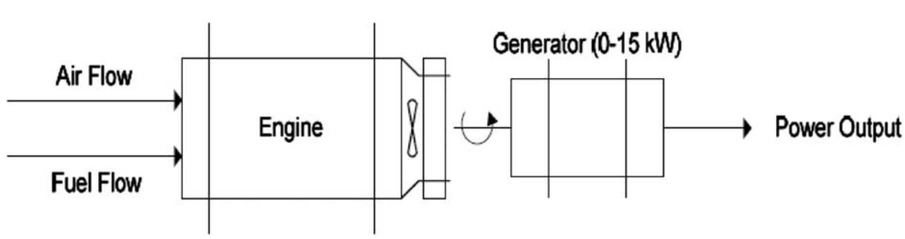

Fig. 1. Schematic of the engine/generator set.