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A Note on Models' Verification, Validation and Calibration

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Abstract

Mathematical models have the potential to provide a cost-effective, objective, and flexible approach to assessing management decisions, particularly when these decisions are strategic alternatives. In some instances, mathematical model is the only means available for evaluating and testing alternatives. However, in order for this potential to be realized, models must be valid for the application and must provide results that are credible and reliable. The process of ensuring validity, credibility, and reliability typically consists of three elements: verification, validation, and calibration.

Model verification, validation and calibration are essential tasks for the development of the models that can be used to make predictions with quantified confidence. Quantifying the confidence and predictive accuracy of model provides the decision-maker with the information necessary for making high-consequence decisions.

There appears to be little uniformity in the definition of each of these three process elements. There also appears to be a lack of consensus among model developers and model users, regarding the actions required to carry out each process element and the division of responsibilities between the two groups.

This paper attempts to provide mathematical model developers and users with a framework for verification, validation and calibration of these models. Furthermore, each process element is clearly defined as is the role of model developers and model users.

In view of the increasingly important role that models play in the evaluation of alternatives, and in view of the significant levels of effort required to conduct these evaluations, it is important that a systematic procedure for the verification, validation and calibration of mathematical models be clearly defined and understood by both model developers and model users.

Keywords: Models, Mathematical Models, Verification, Validation, Calibration.

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Introduction

Different scientific disciplines have defined the terminology in developing, verifying, validating and calibrating their respective mathematical models. However, there appears to be a lack of consensus among model developers as to the terminology to be used in the model development. Because mathematical errors can eliminate the impression of correctness (by giving the right answer for the wrong reason), verification should be performed to a sufficient level before the validation activity begins. The objective of this paper is to provide model developers and users with a more general standard for mathematical modeling.

The model can be divided into a conceptual model and a mathematical model. Ideally, the model developer and experimenter co-develop the conceptual model. Developing the conceptual model involves identifying the objective, the required level of outcomes, the domain of interest, all important physical processes and assumptions, the failure mode of interest, and the validation metrics (quantities to be measured and the basis for comparison). Once the conceptual model is developed, the model developer constructs the mathematical model, which is a set of mathematical relationships intended to describe physical reality (Benekohal, 1991), and designs the validation experiment.

For example, in mechanics, the mathematical model includes the conservation equations for mass, momentum, and (sometimes) energy, the specification of the spatial and temporal domain, the initial and boundary conditions, the constitutive equations, and the relationships describing the model's uncertainty (Oberkampf and Trucano, 2007). In management, the mathematical model consists of budget limitation, resource constraints, balanced equations for diverse stages between the work-load stations and some other limitations which are necessary to be existed for the problem, such as demand inequalities (Maddah et al., 2010).

This paper has four specific objectives:

1. Define a standard description in model verification, validation and calibration.
2. Establish a framework for the systematic verification, validation and calibration of mathematical models.
3. Distinguish between the role of the mathematical model developer and the

model user in the verification, validation and calibration process.

4. Demonstrate the need to develop a standard framework for mathematical model validation.

Definition of the Verification, Validation and Calibration

Typically, developers create models and perform initial model evaluations to provide model users with a level of assurance that the model is reliable and realistic. Model users typically need to select values for input parameters that reflect the specific conditions to be modeled. In addition, model users often desire, or are required, to demonstrate that the model results are realistic and credible.

The first hurdles that model developers and model users must overcome is the acceptance of a standard set of terminology to describe verification, validation, and calibration. Currently, the terms verification, validation, and calibration are often poorly understood and misused or used out of context by modelers (Maropoulos and Ceglarek, 2010). The objective of this section is to propose a standard clear definition to these processes in order to address the misuse of this terminology.

Model Verification

Model verification is defined to be the process of determining if the logic that describes the underlying mechanics of the model, as specified by the model designer, is faithfully captured (AIAA, 1998). Model erification therefore determines if, independent of the logic or the theory from which the logic is derived, can produce the desired outputs. In other words, verification is the process of determining if the modeling logic produces the desired output for a given set of input data. A model is considered to be successfully verified if the model results are consistent, in terms of accuracy, magnitude and direction, with results from the direct application of the logic on which the model is based (Solanki et al., 2010). Therefore, verification is concerned with identifying and removing errors in the model by comparing numerical solutions to analytical or highly accurate benchmark solutions (Roach, 1998). In general, verification deals with the mathematics associated with the model (Shabi and Reich, 2012). For example, if the model designer specifies that $A = B +$ C, then model verification determines if the model computes A as the sum of B and C. Model verification does not attempt to determine whether this relationship adequately captures reality or if A should be equal to something other than the sum of B and C. It should be noted that the level of accuracy is defined by the model developer and is generally a function of the model component that is being verified (James et al., 2010).

Verification does not require that the actual logic, on which the model is based, be accurate in capturing the relevant theory, nor does it require that actual field data be used as input to the model (Pitkaranka et al., 2012). Consequently, verification can be performed independent of field data and without a comprehensive understanding of a practice. However, field data should be considered in order to ensure that the verification is performed for a range of input parameter values, and input parameter combinations, that are consistent with typical field conditions.

Model verification has two objectives:

1- Ensure that, for a given input, the model output are consistent with the current situation which means the model should not produce unexpected results.

2- Conduct limited sensitivity testing to verify that outputs are consistent over the range of typical input values.

Model Validation

Validation is the process of determining the degree to which a theory, an approach or a model is a “good enough” representation of the reality from perspective of the intended uses of the theory, the approach or the model (Anderson and Bates, 2001; Gass 1993; Landry and Oral, 1993). Validation is concerned with quantifying the accuracy of the model by comparing numerical solutions to experimental data. In short, validation deals with the physics associated with the model (Roach, 1998). Validation is a complex process because the concept of “good enough” includes subjective judgments of what constitutes a reasonable degree of a “good enough” and it differs from the point of views of different individuals. Subjective judgments prevent to make a general validation approach of theories, approaches, or models. Therefore, absolute validation is philosophically impossible because it requires not only to eliminate the effects of subjective judgments, which are impossible, but also it needs an infinite number of tests (Anderson and Bates, 2001).

It should be noted that scientific theories cannot be proven; they can only be tested through observations. An agreement of observations with predictions does not validate the theory, but once an exception is observed, the theory is judged to be invalid (Babuska and Oden, 2004). Thus, a theory, a methodology, an approach or a mathematical model can never be proven to be valid; rather, we can say that there are not enough evidences to reject them. Therefore, as long as a methodology or an approach does not have sufficient evidences to reject it, we can accept it.

Validation relative to a specific series of tests may be perfectly legitimate as a basis for making decisions (Babuska and Oden, 2004). In these situations, the relative validation can be possible when validation involves comparison of observed events with those predicted by methods (Kaskonas and Zilinskas, 2010). If an approach or a model has ability to produce more information that would be of value to the decision maker, then the approach or the model is good enough to predict the outcomes of an event (Gass, 1993). Although there are no universal criteria for validation because any validity judgment involves beliefs which are different from one stakeholder to another (Landry and Oral, 1993) but Gass (1993) suggested the validation can be made by theoretical validity, input data validity, and operational validity criteria. However, simplicity, transparency, flexibility, and some sort of criteria that measure the degree of conformity of the model to empirical facts are other types of criteria (Dery et al. 1993).

Model validation attempts to determine if the hypothesized relationship between the underlying behavioral rules and the consequent emergent behavior can be demonstrated to be consistent with the prevailing theory and field data (Cabot et al., 2010). In other words, model validation is considered to be the process of determining to what extent the model's underlying fundamental rules and relationships are able to adequately capture the targeted emergent behavior, as specified within the relevant theory and as demonstrated by field data (Chakraborty et al., 2011). Model validity checks whether or not the proposed model does what it is supposed to do. In other words, validity checks whether the model has the ability to provide a reasonable prediction of the behavior of the system under study (Taha, 2010). In other words, the model is valid if, under similar input conditions, it reproduces past performance. However, there is no assurance that future performance will continue to duplicate past behavior.

Model validation should be done by the model developer and should ideally not be repeated by the model user. Model users should only need to calibrate the model to their particular set of local conditions and need not repeat the validation exercise in order to estimate the expected level of modeling error.

There are three objectives to the model validation:

1- Provide measures that reflect the model's ability to match the selected benchmark (analytical solution or field data) for a particular application domain.
2- Provide a sample of default parameters, together with the range of inputs, for which the validation is applicable.
3- Provide the results of a sensitivity analysis of the model regarding the default parameters in order to indicate the potential rate at which the error increases for a given error level.

For models validation, one should note that all models are approximations of the reality and so they cannot be fully validated. Therefore, rather than think of models as something to accept or reject, it may be more useful to think of models as tools to be modified in response to knowledge gained through continued observation of the natural systems being represented (Anderson and Bates, 2001). We do not know enough about complex natural or human systems to be able to predict them reliably. Mathematical model of a problem, which is the system of related mathematical expressions that describe the essence of the problem (Hilier and Lieberman, 2005), is not an exception in this rule. The model should be a representative of reality. Approximations and simplifying are basic assumptions for constructing a model because it is an abstract idealization of the problem (Hilier and Lieberman, 2005). Therefore, care must be taken to ensure that the model remains a valid representation of the problem

(Scigliano et al., 2011). Model validation regardless of whether or not they are possible, are necessary activities in order to allow models to be used in practical applications. We can think of model input as falling into three categories: factors that are known and measured, factors that can be estimated based on informed judgments (e.g. based on prior experience judgment in systems that are believed to be similar), and guesswork. All models involve informed judgment and typically a bit of guesswork as well. Wherever subjective judgments are required, the potential exists for systematic error and bias.

Model Calibration

Model calibration is considered to be the process of determining to what extent the model user is able to, or is required to modify the default input parameter values, that describe the underlying mechanics, in order to obtain the better values of the problem. Obviously, this process is not easy, because changing a value, for example, needs to change the machineries' technology. In this paper, calibration is defined as the process of selecting the best set of model input parameters to address the most important differences between the model's default assumptions/conditions, and those actually observed locally.

Ideally, calibration consists solely of determining values of input parameters on the basis of available field data. Unfortunately, it is difficult to determine the success or failure of the calibration process by strictly examining the field data and the selected input parameter values because input parameters are incompletely known and there may be unknown effects on the model. All models involve parameters or processes that are known or poorly known, and many models involve the problem of estimating unlike events (Dahmani et al., 2011). In the case of parameters that are poorly known, model developers may take a "best-guess" approach. Lacking quantitative data on a parameter, they make a best assessment of what it might be. However, the accuracy of the input parameter value often can be evaluated, but the impact of this degree of accuracy on the model is much more difficult to estimate because of existence of many parameters involved in the model.

Model users are often not able to

determine the impact that input parameter values have on the selected model. This may arise from several causes, including a lack of understanding of principles, a lack of understanding of the model, poor model documentation, or a combination of these.

The next section of this paper defines the proposed standard verification, validation and calibration in the modeling context. This section also demonstrates how the verification, validation and calibration processes interact. The objective of this section is to provide the reader with a background prior to discussing the individual verification, validation and calibration elements in detail.

Procedure Framework

The individual tasks of model verification, validation, and calibration interact with each other, requiring that they be carried out in a particular sequence, as illustrated in Figure 1.

Model verification, which is the first element of the process, is the responsibility of the model developer. Model verification entails the mathematical relationship between the variables act in a correct manner, running the model error-free and without excessive parameters approximation.

The verification process can be divided into four sequential steps:

1- Selection of Model Input Parameter Values: The values should be selected so that they encompass the expected domain of application of the model. In this step, each input parameter value is checked independently for consistency with typical field data. For example, consider the verification of a company model which its profit should be maximized and it produces two products, A and B. These products can have a mean, a minimum and a maximum profit value. The coefficients of the mathematical objective function can be any (of these) values, depend on model developer thinking. If the minimum (maximum) coefficients are considered, the minimum (maximum) value of objective function would be expected. If the mean values are chosen, we expect to obtain the average of the model objective function. The other situations can be existed such as a minimum value for product A and a maximum value of product B or vice versa. The model output can be checked with the historical data of the company. For instance, in some past data which the company has not had a good situation, the company's profit can be compared with the minimum values of A and B profit data. Therefore, the initial independent check determines if the values chosen for the A and B profit are each within the typical range exhibited by field data.

2- **Combination of the Selected Input Parameters Consistency Checking**: Following the initial independent check for consistency, an additional check is made to test if the combination of the selected model input parameter values is consistent with field data. For example, producing two items A and B which use a single machine, the machine capacity distributed between two items. However, the field data is for producing two items separately by this machine. In other words, both values are separately consistent with the field measurements, together would not be consistent with field data. Thus, the joint assessment ensures that the combination of selected model input parameter values is consistent with typical field data values.

3- **Obtaining Results for the Chosen Input Parameters:** In this step, results are obtained by the solution procedure for the selected input parameters. If the model well formulated, the model will have a solution which is consistent with the current situation, means that there is no any unexpected result (Taha, 2010; Hilier and lieberman, 2005). It is worth noting that the model developer should be convinced that the output of the model does not contain "surprises."

4- **Comparing the Model Output to the Real Output:** This step consists of comparing the model outcome to the real situation when it is possible (Taha, 2010; Hilier and lieberman, 2005). The outcome should make sense and the results should be intuitively acceptable. If the results are within the level of accuracy specified by the developer, the verification process is considered successful. Otherwise the model requires modifications and the verification process must be repeated with the modified model. Because models are usually based on careful examination of past data, the proposed comparison should be favorable.

Model validation, which is also the responsibility of the model developer, is initiated once model verification that been successfully completed. A failure in validation requires that some modifications be made to the model, and thus the verification process must be repeated (Christopher et al., 2011). The iterative cycle is conducted by the model developer until the validation process is successful. At this point the model developer has fulfilled his/her obligations in providing a model that has been successfully verified and validated. It must be emphasized that it is impossible to conclusively demonstrate that a model is valid, since it is impossible to execute the model for every possible combination of input data. Instead the model developer demonstrates that the model is not invalid for the scenarios studied. Care must be taken to ensure that the scenarios that are studied are representative of typical scenarios for which model users are expected to encounter.

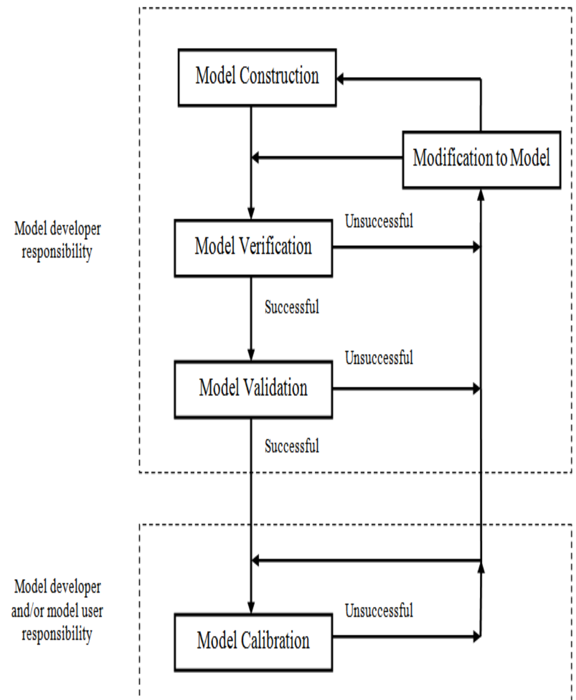

Fig 1 Model verification, validation, and calibration particular sequence.

Validation process can be performed in four steps, which are divided into two groups, defined by analytical validation and field validation. Analytical validation, which is conducted first, examines simple problems in which interaction effects can be limited and for which analytical solutions can be obtained. Subsequently, field validation is conducted, in which an actual real-world problem is modeled, and model results are compared to field data.

Step 1: In this step, a comprehensive suite of strategic hypothetical scenarios are defined, each of which is designed to test a specific model feature. The suite of scenarios must be sequenced so that the most fundamental elements of the model are tested first. The design of this suite of scenarios is critical to the success of the analytical validation process. For example, step 1 in a linear programming model can be done by adding the constraints in a sequential manner to test which of the constraints is critical to the problem.

Step 2: This step consists of the generation of model results and analytical solutions for each of the scenarios in turn. Care must be taken to ensure that assumptions made by the analytical solution are identified, and if possible, captured in the model by the selection of appropriate input parameter values. In the event that several analytical techniques are available, each should be used to generate solutions for comparison to the model results. Furthermore, the results of the model can be compared to the results of other validated models.

Step 3: In step 3, analytical results are compared. The degree of similarity is quantified and the cause of any discrepancies identified. This process is critical, since it clearly identifies the capabilities and limitations of the model. As such, this process requires a comprehensive understanding of the model, the analytical techniques employed to solve the problem, and its theory. In the event that the comparison is unsuccessful, the developer has to make modifications to the model and return to the verification process.

Step 4: This step comprises field validation, which parallels analytical validations with four significant differences.

1- The scenarios examined are actual real-world problems, with the result that model components cannot be examined in isolations and higher order iteration effects cannot be controlled for.

2- The state of the problem is not determined from analytical solutions, but from field data, which must be collected.

3- The generation of model results first require that input parameter values be calibrated using the collected field data.

4- The comparison of model results and field data often provide little insight into the accuracy and applicability of the model. Discrepancies can result from incorrect input parameter value selection (i.e. calibration), or from a fault with the underlying model logic, or both. The developer must discern the cause of the discrepancy and then make the relevant modifications to the model and/or to the calibration of the input parameters. Even if the discrepancies between the model results and the field data are very small, it is possible that compensating errors in the selection of the input parameter values may mask fundamental flaws in the model logic.

Model users, prior to applying the model to their study, must engage in a calibration exercise. The model calibration consists of changing selected input parameter values that cause the best output of the model (Coleman and Steele, 1989). This procedure in a mathematical model can be done by sensitivity analysis. In this analysis, one can change a parameter that guess have the most effect on the solution. The procedure can handle more than one input parameter, but it is complex to recognize which of the input parameters changes can obtain the appropriate result for the model. Three causes can be identified that can lead to an unsuccessful model calibration.

1- Input parameter values may not have been approximated correctly from the existing field data.

2- Insufficient field data or data insufficient quality may have been used to estimate the parameter values.

3- The underlying model logic may be inadequate to capture some behavior phenomena. Unfortunately, it is not generally clear which one, or more, of these factors causes this discrepancy with the model conditions.

Conclusions

This paper has attempted to define a standard description for the verification, validation and calibration of the mathematical models from perspective of model developers and model users. This proposed standard could serve to provide some consensus among model developers and users as to the terminology to be used in model development, testing, calibration and application.

Model verification, validation and calibration are the primary processes for quantifying and building credibility in numerical models (Schlesinger, 1979). Verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and its solution. Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. Both verification and validation are processes that accumulate evidence of a model's correctness or accuracy for a specific scenario. Calibration is process of adjusting numerical modeling parameters for the purpose of improving the model's result. This process is a complex task because there may be some huge parameters involved in the real-world problem and its associated model. Therefore, recognizing which of the parameters have the most effect on the model is very hard. This process cannot prove that a model is correct and accurate for all possible scenarios, but, rather, it can provide evidence that the model is sufficiently accurate for its intended use.

The paper has established a systematic framework for the verification, validation and calibration procedure of mathematical models. Furthermore, the paper has also defined the role of the model developer and user. The model developer should be responsible for conducting the model verification and validation exercises. In one hand, the model developer should describe how much a model can describe well the current situation, together with a description of the different input parameters, their impact, acceptable ranges, and default values. On the other hand, the model user should be responsible for calibrating the model input parameters to the field data. It should be noted that the model developer should provide documentation describing validation tests that have been conducted. This can be done by a comparison between the model outputs with current output.

It is recommended that a standard calibration framework be developed to assist users in the calibration of the models. This framework should provide the user with some strategies to be utilized in order to address different calibration issues.

In general, given the diversity of human attitudes and opinion, one might hope that individual bias and unusual feature would happen when making the models. For example, construction of more than one model of a system can reveal biases and errors in a single model. Different model developers or groups of them may have different subjective tendencies, and the totality of independently constructed models might converge on a correct result. A fundamental issue in making the models is the problem of non-uniqueness: more than one model may produce different outputs. Under common operational definitions of validation, one may declare a model validated while another may use the same data to demonstrate that the model is invalid. There is no way to eliminate subjectively and value judgment and therefore, we cannot and do not expect any model to be precisely validated in all respects.

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یادداشتی در مورد راستی‌آزمایی، اعتبارسنجی و تنظیم مدل

علی خاتمی فیروزآبادی[1]

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مدل‌های ریاضی از این توانایی برخوردارند که می‌توانند یک رویکرد هزینه‌ای، هدفمند و انعطاف‌پذیر موثر را به منظور ارزیابی تصمیمات مدیریتی، به ویژه هنگامی که این تصمیمات از نوع گزینه‌های راهبردی باشند را فراهم آورند. در برخی از موارد خاص، فقط از مدل‌های ریاضی می‌توان برای ارزیابی و آزمایش گزینه‌ها استفاده کرد. مثلاً آزمایش‌هایی که خطراتی را به علت وجود اسیدهای مایع در پی دارد به توسط قانون ممکن است ممنوع شده باشد و لذا در این‌گونه مواقع، مدل‌سازی ریاضی تنها راه چاره برای ارزیابی عملیات در این نوع فرآیندها به شمار می‌رود. به منظور استفاده درست از مدل‌ها، لازم است نه تنها مدل‌ها از اعتبار برخوردار باشند بلکه نتایجی که حاصل از به‌کار گیری آنهاست قابل اتکا و قابل اعتماد باشد. فرآیندی که اعتبار مدل، قابلیت اتکا و همچنین قابلیت اعتماد به آن را به دنبال دارد دربردارنده سه عنصر راستی‌آزمایی، اعتبارسنجی و تنظیم مدل است.

راستی‌آزمایی، اعتبارسنجی و تنظیم مدل از جمله مواردی است که باید در گسترش مدل‌ها مورد توجه قرار گیرد. در این صورت است که می‌توان با اطمینان از مدل‌ها برای پیش‌بینی‌ها استفاده کرد. کمی کردن اطمینان و دقت در پیش‌بینی مدل برای تصمیم گیرنده شرایطی را به وجود خواهد آورد که بتواند با

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۱. دانشیار دانشکده کسب و کار دانشگاه علامه طباطبایی.

اطلاعات لازم، تصمیمات مناسب را با اطمینان بالا اتخاذ کند.

مطالعه ادبیات مربوط به این سه فرآیند، نشان می‌دهد که اختلاف نظرهایی در تعاریف مربوط به این سه فرآیند وجود دارد. همچنین مشاهده می‌شود که اتفاق نظری در خصوص انجام این فرآیندها و حتی عملیات مورد نیاز هر فرآیند، بین مدل‌سازها و کاربرانی که از مدل‌ها استفاده می‌کنند نیز وجود ندارد.

در این مقاله سعی می‌شود چارچوبی برای راستی‌آزمایی، اعتبارسنجی و تنظیم مدل‌های ریاضی، هم برای گسترش دهندگان این نوع مدل‌ها و هم استفاده کنندگان از آنها را فراهم آورد. علاوه بر آن، سعی می‌شود تا عناصر سه‌گانه مزبور به‌روشنی تعریف شود و نقش گسترش دهندگان مدل و کاربران مدل را معین سازد.

نوعاً گسترش دهندگان، مدل‌ها را ساخته و ارزیابی‌های اولیه‌ای برای آن ارائه می‌دهند تا بتوانند استفاده کنندگان را با سطحی از اطمینان متقاعد سازند که مدل ساخته شده، قابل اعتماد است و می‌تواند واقعیت را دربرگیرد. استفاده کنندگان از مدل‌ها معمولاً مقادیر خاصی را به عنوان پارامترهای ورودی به مدل انتخاب می‌کنند تا عکس‌العمل مدل را نسبت به این پارامترهای خاص بسنجند تا ببینند که آیا مدل ساخته شده قادر به تشخیص موارد خاص بوده است یا نبوده است. به‌علاوه، استفاده کنندگان از مدل‌ها، اغلب نتایج حاصل از مدل‌ها را با شرایط واقعی مقایسه می‌کنند تا درجه تطبیق آن را با واقعیت بسنجند.

با توجه به نقشی که مدل‌ها در ارزیابی گزینه‌های تصمیم‌گیری دارند و همچنین با توجه به تلاش‌های بسیار زیادی که برای ساخت مدل‌ها می‌شود داشتن رویه‌ای نظام‌مند که بتواند مقوله‌های راستی‌آزمایی، اعتبارسنجی و تنظیم مدل را به‌روشنی تعریف کند و به توسط گسترش دهندگان مدل‌ها و هم استفاده کنندگان از آنها درک شود حائز اهمیت است.

واژگان کلیدی: مدل، مدل‌های ریاضی، راستی‌آزمایی، اعتبارسنجی، تنظیم مدل.