Construction of adequate mathematical model of physical object from merit function

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Abstract. Methodology for construction of adequate mathematical model of the object from merit function is proposed. Characteristics which determine degree of acceptability of the model are introduced: acceptable disagreement between modelling results and experimental data, required number of states of the object of study, significance thresholds of independent variables. Software package for construction of adequate mathematical model has been designed which allows us to automate the construction process. Proposed methodology and software package allow for transition to mathematical model with given in advance disagreement between modelling result and experimental data. The degree of acceptability of already existent mathematical models can also be improved.

1. Introduction
Scientific study of physical object usually is based on its mathematical model. Therefore, it is important that its degree of acceptability allows to obtain satisfactory result, where the researcher provides acceptable percentage of disagreement between modeling results and experimental data, and where degree of acceptability shows relative difference between actual and permissible disagreement.

The object of study can be described by merit function of dependent and independent variables, where independent variables are understood to be random values with given tolerance intervals and distribution laws (uniform, normal and other).

In order to transit from merit function to adequate mathematical model it is necessary to determine for each independent variable its absolute and relative relevance and its maximal influence coefficient. Next the number of their representative values, their distribution within uncertainty intervals, their entropy and significance are determined.

Significance threshold is given by experts and those independent variables, which significance is below given threshold, are represented by constants in mathematical model as arithmetic mean within corresponding interval. Those of independent variables which significance is above the threshold are described in the model by distribution of representative values (model parameters) within independent variable's uncertainty interval.

Thus, we obtain parametrized mathematical model which variables are dependent variables of the merit function.

In transition from the merit function to mathematical model its degree of acceptability can be increased by varying required number of states of the object $N_{req}$, significance threshold of each independent variable and allowable disagreement between modeling results and experiment.

Several articles [1, 2, 3] were found during reviewing bibliographical and referential databases
where families of merit functions are considered but none of them talks about transition from merit function to mathematical model.

2. A method for construction of adequate mathematical model of physical object from merit function.

Let merit function be
\[ y = y(z_p, x_w) \]
where \( x_w = (x_1, ..., x_m, ..., x_L) \) is a vector of independent variables and \( z_p = (z_1, ..., z_k) \) is a vector of dependent variables. Here each dependent variable \( z_i \) can be given by several values of \( z_{11} \ldots z_{1k} \).

Similarly each independent variable, for example, \( x_m \), can take several random values \( x_{mj}, j = 1, ..., n_m \) within given allowable range or domain \( \min_j x_{mj} \leq x_{mj} \leq \max_j x_{mj} \).

Let us determine how independent variable \( x_m \) influences the value of the merit function, but initially we will be limited only by one dependent variable \( z_l \). Later, all dependent variables will be considered.

In order to elucidate this influence, we will suppose that other independent variables take arithmetic mean values \( x_{avgl}, l = 1, ..., L, l \neq m \) within their intervals. The influence of uncertainty domain of independent variable \( x_l \) is determined by absolute relevance
\[
Ra_{im} = \frac{\max_j (x_{lj}x_{cp1}, ..., x_{lj}x_{cpL})}{y(x_{lj}x_{cp1}, ..., x_{lj}x_{cpL})} - \frac{\min_j (x_{lj}x_{cp1}, ..., x_{lj}x_{cpL})}{y(x_{lj}x_{cp1}, ..., x_{lj}x_{cpL})}
\]  

Next for independent variable \( x_m \) and given value of dependent variable \( z_l \) we determine the influence coefficient or relative relevance:
\[
Rb_{lm} = \frac{Ra_{im}}{\sum_{l=1}^{L} Ra_{il}}
\]

We found then maximum of influence coefficient of independent variable \( x_m \) by cycling through all the values of single dependent variable \( z_l \) and repeating each time the calculation of influence coefficient or relative influence:
\[
R_m = \max_l Rb_{lm}
\]

Similarly in order to take into account all of the dependent variables \( z_1 \ldots z_k \), each of which is determined by several values, all the sets of different values of dependent variables are cycled and for each case all the previous calculations are done and finally the maximum of influence coefficient of independent variable \( x_m \) is obtained.

In the same way maximal values for each of the influence coefficients of independent variables are found.

Significance of independent variable \( x_m \) is given by equation:
\[
B_m = R_m \times H_m
\]

where \( H_m \) is an entropy of independent variable \( x_m \) which determines its informativeness, so to obtain the value of significance of the independent variable its entropy also needs be found.

In our case independent variable \( x_m \) is continuously distributed within the given range with given probability density function \( f_m(x) \). For this case entropy can be calculated with approximate expression
\[
H_m(\Delta_m) = -\int_{-\infty}^{+\infty} f_m(x) \times ln f_m(x) dx - ln\Delta_m
\]
Here the first addend describes influence of probability distribution given by probability density function \( f_m(x) \) on the entropy of \( x_m \). Second addend \((- \ln \Delta_m)\) considers discretization interval \( \Delta_m \).

If for entropy equation we substitute \( f_m(x) \) with probability density function for uniform or normal distribution we get

\[
H_{\text{equ}}(\Delta_m) = \ln \left( \frac{\text{max}_j x_{mj} - \text{min}_j x_{mj}}{\Delta_m} \right) \quad \text{for uniform distribution}
\]

and

\[
H_{\text{norm}}(\Delta_m) = \ln \left( \frac{2 \pi e \sigma^2}{\Delta_m} \right) \quad \text{for normal distribution. Here } \sigma \text{ is a normal distribution parameter.}
\]

In order to find representative values \((NW)\) of independent variables it is necessary to solve a problem of optimal decision making: representative value for each independent variable should be chosen in such a way that transition from merit function to mathematical model is adequate (precise), but the number of representative values is as small as possible in favor of computational cost reduction.

Let us consider one of the ways to solve the problem.

Let \( L \) be the number of independent variables \((x)\) and \( N \) – the number of all the combinations of representative values of independent variables. That is \( N \) is the number of possible states of the object. Then

\[
N = \prod_{t=1}^{L} (NW_t)
\]

Next the number of representative values \( NW_m \) of independent variable \( x_m \) is considered proportional to its significance \( B_m \):

\[
NW_m = P \times B_m
\]

Here \( P \) is a proportionality constant which is same for all independent variables.

If significance is represented by maximal value of influence coefficient of independent variable \( x_m \) and its entropy, we obtain \( NW_m = P \times R_m \times H_m \). But the entropy also depends on the number of representative values \( NW_m \) via \( \Delta_m \) – the length of partition interval of finite domain of distribution function of independent variable \( x_m \). This gives an equation where \( NW_m \) is unknown and which is to be solved for each independent variable.

For this we initially limit probability density function \( f_m(x) \) within finite domain \((b)\) and let \( \Delta \) be constant for every independent variable:

\[
b = \Delta \times NW
\]

On the other hand, according to assumption of normal distribution \( b_{\text{norm}} = 6\sigma \) and thus

\[
\sigma = \frac{(\Delta \times NW)}{6}
\]

By substituting expression for \( \sigma \) in entropy formula for normal distribution we obtain

\[
H_{\text{mnorm}} = \ln \left( \frac{NW}{6} \times \sqrt{2\pi e} \right) = \ln(NW) + h_{\text{norm}}
\]

here \( h_{\text{norm}} \) is differential entropy for normal distribution which computes as \( h_{\text{norm}} = -0.3728 \).

Differential entropy values for other distributions can be computed similarly according to their parameters.

So, to obtain entropy and significance for each independent variable its representative value \((NW)\) needs be found.

For this purpose, knowing differential entropy values of distribution of independent variables experts provide required number of states of the object which are to be considered.

By giving \( N_{\text{req}} \) as the product of the amount of representative values of all independent variables
their values are determined. First, independent variable with minimal relevance is selected. Let it be \((x_m)\). For this variable the number of representative values \(NW_m\) is assigned in advance. Next from expression \(NW_m = P \times R_m \times H_m\) value of \((P)\) is determined. Thereafter in place of \((H_m)\) its value \(H_m = \ln(NW_m) + h_m\) represented via differential entropy is substituted. Knowing that proportionality constant \(P\) is the same for all independent variables \((P_m = P_l = P)\) an equation is obtained, out of which supplying the number of representative values \((NW_m)\) of one independent variable \(x_m\) representative values \((NW_l)\) for other independent variables \(x_l\) can be found. This equation is given as

\[
\frac{NW_m}{(\ln(NW_m) + h_m) \times R_m} = \frac{NW_l}{(\ln(NW_l) + h_l) \times R_l}
\]  

(10)

Here where \(NW_m\) is given and \(h_m, R_m, h_l, R_l\) are determined we have the only unknown \((NW_l)\) which is the number of representative values for independent variable \(x_l\). Every time by cycling through all the independent variables this equation is being solved by substituting by corresponding values of the differential entropy \((h)\) and the maximal value of influence coefficient \((R)\). As a result, the number of representative values \((NW)\) for all independent variables \((x)\) is found. After that product of all their \((NW)\) is computed and compared to \(N_{req}\) given by experts. If the result is below \(N_{req}\), the number of representative values \((NW_m)\) for independent variable \((x_m)\) with the lowest relevance is increased and computation of amounts of representative values \((NW)\) is repeated until the result is above \(N_{req}\), in which case the amount of representative values \((NW)\) from previous calculation is taken as obtained for all the independent variables \((x)\).

Then we substitute them alongside with values of corresponding differential entropy in equation \(H = \ln(NW) + h\) to obtain significance for all the independent variables and transit from the merit function to mathematical model.

The distribution of representative values \((NW)\) of all independent variables \((x)\) within their uncertainty domains \(\text{min}_j x_j \leq x_j \leq \text{max}_j x_j\) or of the mathematical model parameters are obtained by satisfying the condition that their probabilities must correspond to the given probability density functions \(f_m(x)\) of these independent variables.

By varying input data \(N_{req}\), significance thresholds and redefining type of adequate model one obtains acceptable agreement of modeling result and experiment. At the same time obtained input data determines degree of acceptability of the mathematical model.
3. **Software package for construction of adequate mathematical model**

Figure 1 depicts architecture level of software package for construction of adequate mathematical model (SPCAMM).

![Figure 1](image-url)

**Figure 1** Architecture level of software package for construction of adequate mathematical model.
4. Conclusion
Proposed methodology and software package allow for transition from merit function to mathematical model with given in advance disagreement between modeling result and experimental data. The methodology utilizes methods of calculation of quantitative properties based on decision making theory.

With the help of proposed methodology and the software package the degree of acceptability of already existent models can be improved. In work [4] a transition from mathematical model to merit function is described but it does not correspond to the proposed one which uses calculation of quantitative properties based on decision making theory.

Presented architecture of software package for construction of adequate mathematical model and its developed prototype allows automation of model construction.

Software package prototype has been implemented in Python programming language. Source code contains 4361 lines, defines 35 classes in 19 files. Comments occupy 1613 lines (37%).

References
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