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POLYNOMIALS IN METAMODELING OF GLASS FIBRE BAR STABILITY

POLINOMI STIKLŠĶIEDRAS STIEŅU STABILITĀTES METAMODELĒŠANĀ

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Polynomial regression, metamodeling, subset selection, basis function construction, heuristic search

1. Introduction

Computation-intensive design problems are becoming increasingly common in manufacturing industries. Despite the advances in computer capacity and speed, the enormous computational cost of complex, high fidelity scientific and engineering simulations makes it impractical to rely exclusively on simulation for the purpose of design optimization. To cut down the cost, metamodels, also known as surrogate models, are constructed from and then used in place of the actual simulation models [1,2,3]. Metamodeling techniques have been widely used for design evaluation and optimization in many engineering applications.

The primary objectives of metamodeling are to obtain an accurate estimate of the response and to minimize the required computational effort [2]. This includes minimizing the necessary number of sample points and utilizing a computationally efficient modelling method which creates models of high predictive performance.

Typically, in metamodeling a low-order polynomial model is used – usually a second-order polynomial [2]. A low-order polynomial has a low number of unknown parameters and tends to smooth out noise in the data. However, it cannot model highly nonlinear behaviours. Higher-order polynomials can be used, but instabilities may arise as higher order polynomials can exhibit erratic behaviour in the sub-domains not covered by the experiments [4,5,6], or it may be too difficult to take sufficient sample data to estimate all of the parameters in the polynomial equation, particularly in large dimensions [6].

As a possible remedy for the problem, subset selection techniques [7,8,9] may be used. They are aimed to identify the best subset of basis functions to include in the regression model, and to remove the unnecessary ones (e.g., by using the statistical significance tests [7,8,9] or information-theoretic criteria such as the Akaike's Information Criterion (AICC) [10]).

Before the subset selection step one chooses the maximal order, of the resulting polynomial, in this way creating a *fixed* finite set of predefined basis functions which will be used in model building. Then the actual subset selection is performed. The goal is to find a subset that maximises the predictive performance of the resulting regression model.

In order to find the subset of basis functions, some kind of search must be performed. The simplest search strategy is the exhaustive search, which evaluates every possible subset. Although exhaustive search guarantees to find the best subset (according to evaluation criterion used), it needs exponential runtime and thus is impractical in most cases.

Another class, called heuristic search methods, efficiently traverse the space of subsets, by adding and deleting the basis functions, and uses an evaluation function that directs the search into areas of increased performance. The typical examples of heuristic search methods are the Forward Selection, also known as Sequential Forward Selection (SFS), and the Backward Elimination, also known as Sequential Backward Selection (SBS) [8]. SFS starts with an empty set of selected basis functions (or with the intercept term already included) and iteratively adds the function leading to the highest performance increase to the set of selected functions, until the performance cannot be enhanced any further by adding a single function. SBS starts with the complete set of basis functions and iteratively removes the function whose removal yields the maximal performance increase.

The approach of subset selection assumes that the chosen *fixed* finite full set of *predefined* basis functions contains a subset which is sufficient to describe the target relation sufficiently well. However, in many cases the necessary maximal order of the resulting polynomial (or set of basis functions) is not known and needs to be guessed or chosen by experience. In many cases that means a non-trivial (and long) trial and error process, since it can differ from one data set to another and would also be, for practical reasons, guided by computational complexity issues [12].

A more convenient and potentially efficient approach is to let the modelling method itself construct the basis functions necessary for creating the regression model with adequate predictive performance. This can be done using the so-called Basis Function Construction (BFC) approach [12]. The BFC approach does not require the user to worry about choosing the maximal order (or predefining the set of basis functions). BFC automatically constructs the necessary basis functions using heuristic search, efficiently trading-off the simplicity and predictive performance of the models.

In the paper, we consider application of four different polynomial regression modelling methods to a problem of glass fibre bar stability metamodeling. The four methods include a simple p-th order polynomial regression (PR), SFS with F-statistic, SFS with AICC, and an instance of the BFC approach – a regression modelling method called Sequential Floating Forward Polynomial Construction (SFFPC) [12].

In the following section, we shortly describe the glass fibre bar stability metamodeling study. Next, we describe the four applied polynomial regression modelling methods and shortly discuss their differences and similarities. Finally, we describe the performed metamodeling experiments, show the results, and draw some conclusions about the used methods.

2. Glass fibre bar stability studies

Whenever a structural member is designed, it is necessary that it satisfies specific strength, deflection, and stability requirements. Slender or thin-walled structural members that are subjected to compression are prone to buckling – loss of stability. This possible loss of stability is often the determining factor in design of such members. Axially compressed column is the simplest case here, and analytical and numerical buckling analysis is simple (though it is sufficient for our experimental comparisons of regression modelling methods). For more complicated structures, analytical prediction of buckling load can be impossible and numerical solutions can take much time and even be inaccurate, if used improperly [13]. In this study, axially compressed glass fibre reinforced plastic (GFRP) bar is used. The geometrical design parameters of the considered bar are given in Fig. 1.

The maximum axial load that a column can support, when it is on the verge of buckling, is called the critical load, P_{cr} (see Fig. 1 (a)). Any additional loading will cause the column to buckle and therefore deflect laterally as shown in Fig. 1 (b). In 1757, mathematician Leonhard Euler derived a formula that gives the maximum axial load that a long, slender, ideal column can carry without buckling. An ideal column is one that is perfectly straight, homogeneous, and free from initial stress. The Euler formula for columns is

$$P_{cr} = \frac{\pi^2 EI}{(\mu L)^2},$$

where P_{cr} is critical force; E is modulus of elasticity of the material; I is minimum area moment of inertia of the cross-section; L is unsupported length of column; μ is column effective length factor, whose value depends upon the conditions of end support of the column [14].

In the current study a hollow GFRP column with rectangular cross-section and pinned supports at the ends is considered. The changing parameters are the following: a, kt, kb, L (see Fig. 1 (c)). Analytically P_{cr} can be calculated by Euler formula, where μ = 1 and $I = I_{min}$ is calculated as follows:

$$I_{\min} = \frac{ab^3 - (a-2t)(b-2t)^3}{12}.$$

For this study, a set of numerically obtained results is used. The numerical calculations were performed using Finite Element software ANSYS 11.0 [15,16]. A data set of 300 experiment points in four-dimensional space was conducted, which were sampled using Minimum Square Distance Latin Hypercube [17]. Value intervals of the design parameters are the following: $0.025 \le a \le 0.25$ m, $7 \le kt \le 10$, $1 \le kb \le 3$, $1.0 \le L \le 6.0$ m.

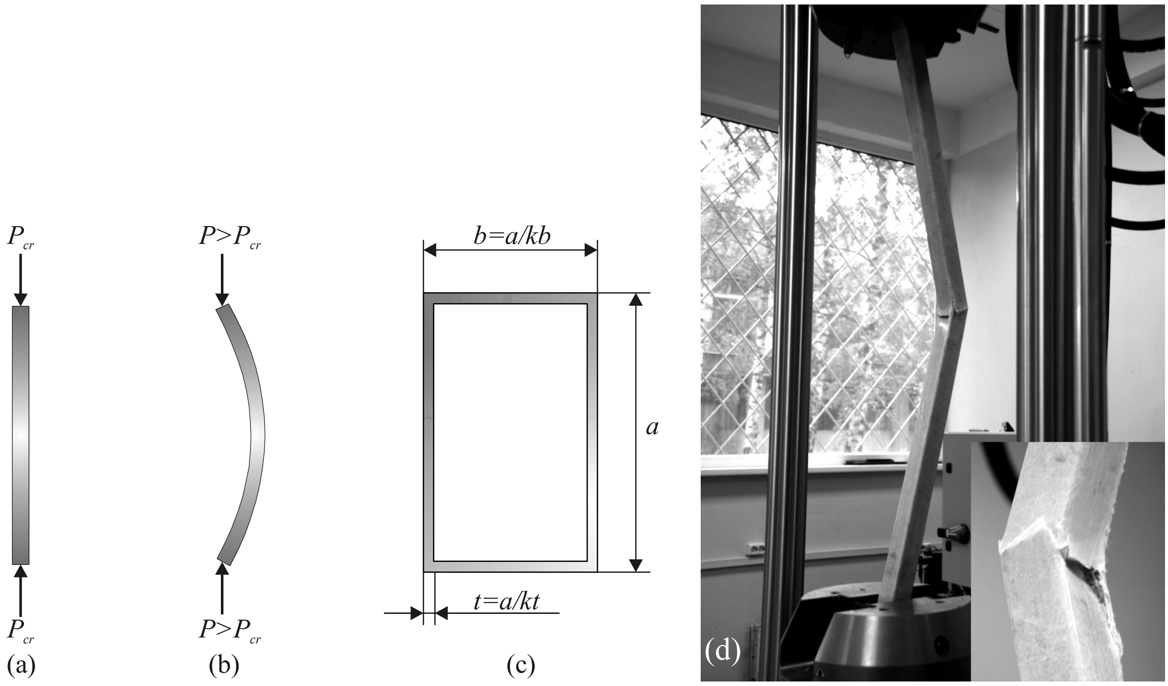

Figure 1. The axially compressed bar. Geometrical design parameters ((a), (b), (c)) and the practical stability test of the bar (d)

3. Polynomial regression modelling methods

In this section, we will describe the four polynomial regression modelling methods used in the metamodeling experiments. Note that, to be strict, the first method, *p*-th order polynomial regression, is generally not a regression modelling method, as there is no model building or searching performed – there is only one a priori chosen model.

3.1. p-th order polynomial regression

A polynomial regression model of order *p* can be expressed as:

$$\hat{y} = a_0 + \sum_{i=1}^{d} a_i x_i + \sum_{i=1}^{d} \sum_{j>i}^{d} a_{ij} x_i x_j + \sum_{i=1}^{d} a_{ii} x_i^2 + \sum_{i=1}^{d} \sum_{j>i}^{d} \sum_{m>j}^{d} a_{ijm} x_i x_j x_m + \ldots + \sum_{i=1}^{d} a_{i,i,\ldots,i} x_i^p$$

where a_i are model's parameters; *d* is the number of the original independent variables. The second order polynomial model is often considered as the synonym of the Response Surface method (e.g., [18] and many other researchers).

Since polynomial regression models are linear in the parameters, the usual linear model tools may be applied – the parameters a_i of the regression models are estimated using the ordinary least-squares method, OLS.

3.2. Sequential Forward Selection with F-statistic

Generally a polynomial regression model may be defined by a linear summation of basis functions:

$$\hat{y} = \sum_{i=1}^{k} a_i f_i(x)$$

where k is the number of the *used* basis functions (equal to the number of model's parameters); and $f(x)$ are the basis functions which generally may be defined as a product of original input variables each raised to some order:

$$f_i(x) = \prod_{j=1}^{d} x_j^{r_{ij}} \quad (1)$$

where r_{ij} is the order of the j-th variable in the i-th basis function (a non-negative integer). Note that when all r_j's of a basis function are equal to 0, we have the intercept term.

Usually in the subset selection the basis functions are chosen such that the order of each possible polynomial model does not exceed a previously chosen highest allowed order p, i.e. each $r_{ij} \in \{0,1,...,p\}$ and $\sum_{j=1}^{d} r_{ij} \leq p$ for all i.

SFS with F-statistic [7,8,9] starts with the simple model with only the intercept term in it and sequentially adds those basis functions to the model that most significantly improve its fit to the training data. To avoid overfitting, the significance of the Mean Squared Error improvement gained by adding the basis function to the current model is tested. The improvement is significant, if the obtained F value is greater than a predefined significance threshold value. SFS proceeds with greedy search by choosing the best significant improvement and stops, if no significant improvement is available.

3.3. Sequential Forward Selection with AICC

Another way of performing model evaluation in subset selection is using the complexity penalization criteria. In contrast to the F-statistic, complexity penalization criteria do not require the compared models to be nested and do not require the user to set the significance threshold value. The most widely known and used complexity penalization criterion is the Akaike's Information Criterion (AIC) [10]. In our research we used its small sample corrected version (AICC) [11]:

$$\text{AICC} = n\log(MSE) + 2k + (2k(k+1))/(n-k-1)$$

where MSE is Mean Squared Error in training data; n is the number of data cases in the training data. Note that the best fitting model is that whose criterion value is the lowest.

SFS with AICC works very similarly to SFS with F-statistic except that it sequentially adds those basis functions to the model that lower the AICC value the most. The process is stopped when no further addition of any basis function can gain decrease of AICC.

3.4. Sequential Forward Floating Polynomial Construction

SFFPC [12] is an instance of the BFC approach – it is a regression modelling method that can by itself construct the necessary basis functions and generate polynomials of arbitrary complexity, efficiently trading-off the simplicity and predictive performance of the models.

In BFC, the standard model refinement operators of subset selection, namely addition (and deletion) of basis functions, are replaced with other operators which not only allow adding or deleting basis functions but also allow changing the basis functions themselves. BFC operates directly with the orders of each variable in each function as well as creates new functions as necessary. Thus in BFC one operates with a matrix of non-negative integers where a cell in *i*-th row and *j*-th column contains a value of r_{ij} in equation (1) which is the order of the *j*-th variable in the *i*-th basis function.

In SFFPC, the starting point of the search is the same as in the two subset selection methods described above – a model with one function that corresponds to the intercept term (this function stays in the model at all times and is not allowed to be modified or deleted).

SFFPC uses five model refinement operators:

- *Operator1*: Increasing of one of the orders in one of the existing basis functions by 1.
- *Operator2*: Addition of a new basis function with one of the orders set to 1.
- *Operator3*: Addition of an exact copy of already existing basis function with one of the orders increased by 1.
- *Operator4*: Decreasing of one of the orders in one of the existing basis functions by 1.
- *Operator5*: Deletion of one of the existing basis functions.

The operators are categorized as *complication* operators (the first three) and *simplification* operators (the last two). In the search process the complication operators do the main job – they "grow" the regression model. The simplification operators on the other hand work as purifiers – they decrease the unnecessarily high orders and delete the unnecessary basis functions. As it may be noticed, the space of candidate regression models is now infinite, and we can generate polynomials of arbitrary complexity.

As a search strategy that of Sequential Floating Forward Selection [19] is used. It consists of applying after each forward step a number of backward steps as long as the corresponding constructed models are better than the previously evaluated ones. The strategy is effective in minimizing the nesting effect and avoiding getting stuck in local minima too early [12,19].

When the complication operators cannot give any further improvements, the search process is not yet stopped. All the candidate models of the current step are additionally modified by using the same refinement operator the second time. If a new better model was created, the search process is continued with the five refinement operators as before. Otherwise the search process is finally stopped.

For a more detailed description of the BFC and SFFPC see [12].

4. Metamodeling experiment

We applied the four regression modelling methods to the above described problem of glass fibre bar stability metamodeling and compared the results. We estimated predictive error of the induced models on unseen data samples using 10-fold Cross Validation (CV) and averaged the results. The predictive performance of a model in test data set is measured in terms of relative root mean squared error, RRMSE:

$$RRMSE = \sqrt{\sum_i (y_i - \hat{y}_i)^2} \Big/ \sqrt{\sum_i (y_i - \bar{y})^2} = RMSE/STD$$

where $\hat{y}_i$ is the corresponding predicted value for the observed value y_i; $\bar{y}$ is the mean of the observed values. While RMSE (Root Mean Square Error) represents model's deviation from the data, the STD (Standard Deviation) captures how irregular the problem is. The lower the value of RRMSE, the more accurate the model.

In the experiments, as implementation of PR, SFS with AICC, and SFFPC we used our in-house software. As implementation of SFS with F-statistic we used the statistical software package STATISTICA 7.0 [20] with its default parameters. For SFS with AICC we varied the maximal polynomial order, p, in interval $2 \le p \le 9$. For PR we varied p in interval $2 \le p \le 6$, as higher values make the number of model's parameters exceed the number of data cases. For SFS with F-statistic the used software only allowed $p = 2$. For SFFPC of course there was no need to set the maximal order.

Table 1. The results for the metamodeling problem.
Average RRMSE error (%), its standard deviation (%), and model complexity *k*

Method	RRMSE	StdDev	*k*
PR, $p = 2$	88.44	37.55	15
PR, $p = 3$	72.09	32.02	35
PR, $p = 4$	48.02	25.40	70
PR, $p = 5$	25.97	12.50	126
PR, $p = 6$	19.33	14.88	210
SFS with F-statistic, $p = 2$	87.31	36.93	10
SFS with AICC, $p = 2$	87.88	36.27	10
SFS with AICC, $p = 3$	76.33	32.48	19
SFS with AICC, $p = 4$	46.45	22.31	34
SFS with AICC, $p = 5$	30.75	13.49	49
SFS with AICC, $p = 6$	16.12	4.96	70
SFS with AICC, $p = 7$	11.69	5.19	86
SFS with AICC, $p = 8$	9.02	4.47	102
SFS with AICC, $p = 9$	11.72	12.38	113
SFFPC	3.46	0.50	99

Table 1 presents the results of the experiment on the metamodeling problem with the four regression modelling methods. It was observed that in this metamodeling problem the highest predictive performance is the property of the high-order polynomials, i.e., the order of the best model obtained using the SFS is eight. In relation to the full polynomials (PR), it was not possible to set such high order as it would make the number of models' parameters exceed the number of data cases. This resulted in underfitting. Moreover the high number of parameters in PR resulted in high standard deviation comparing to the standard deviation of the models built by SFS of the same order.

Overall the instance of the basis function construction approach, SFFPC, here is clearly superior to all the others – it was able to find models with the best predictive performance – the lowest average RRMSE with the lowest standard deviation.

Additionally three-dimensional graphical validations of the obtained regression models for critical load P_{cr} versus bar length L and bar width a, with fixed $kt = 8$ and $kb = 2$, were carried out as presented in Fig. 2. By graphical validation one can easily identify that the best regression models of PR and SFS are not well behaved. On the other hand, the regression model obtained by SFFPC gives the best overall perspective of structural behaviour – its surface looks most alike to the surface obtained by the analytical formula, including also the plateau type region.

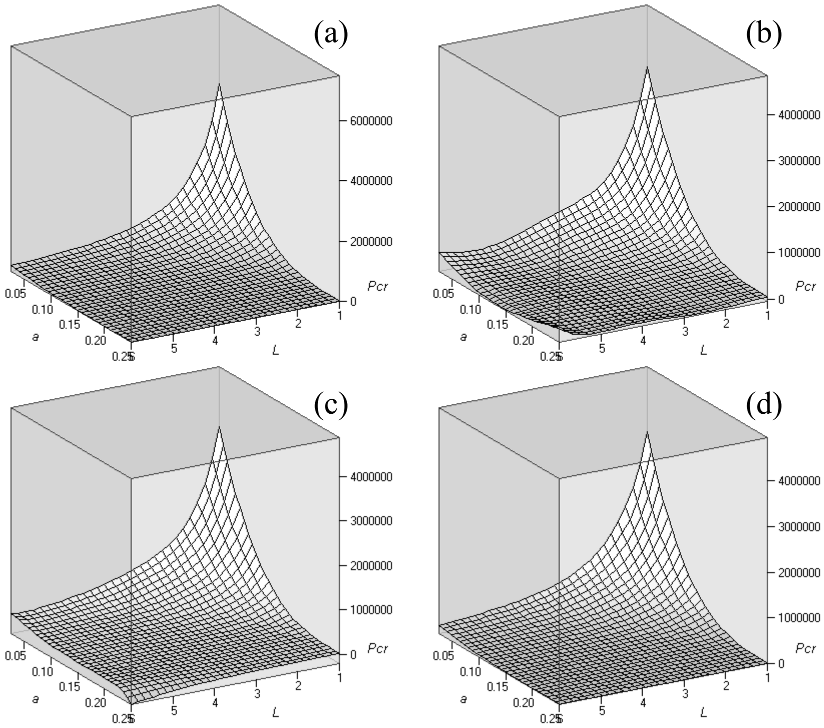

Figure 2. Graphical validation of the best found regression models for the first CV fold. Analytical solution (a), PR with p = 6 (b), SFS with p = 8 (c), and SFFPC (d)

5. Conclusion

It was concluded that in metamodeling of buckling behaviour of structures the basis function construction approach appears to have a potential to efficiently construct regression models of relatively high predictive performance. The obtained models, by their precision, are capable of serving in the development process for design guidelines of new structures.

Moreover the approach does not require the user to guess the maximal order of the models (or predefine the full set of basis functions) as in most other polynomial regression modelling methods. The modelling method itself constructs the basis functions necessary for creating the regression model with adequate predictive performance. This can considerably speed-up the modelling process in practical applications.

Directions of future research include applying the adaptive basis function construction approach also in other types of metamodeling applications to evaluate the proposed approach more generally. The built models also will be used for further (cost/weight) design optimisation studies together with structural sizing studies and parametric sensitivity analysis.

Acknowledgement

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Jēkabsons G., Kalniņš K., Eglītis E. Polinomi stiklšķiedras stieņu stabilitātes metamodelēšanā

Metamodelēšanā tipiski tiek izmantots zemas pakāpes polinoms – parasti otrās pakāpes polinoms. Tomēr tas nespēj modelēt augstas nelinearitātes uzvedības. Var tikt izmantoti augstākas kārtas polinomi, taču tas var izraisīt aproksimanta nestabilitāti. Kā šīs problēmas pretlīdzekli var izmantot apakškopu izvēles metodes. Taču tajās tiek pieņemts, ka izvēlētā fiksētā pilnā iepriekš izvēlēto bāzes funkciju kopa satur apakškopu, kas ir pilnīgi pietiekoša sakarību pietiekoši labai aprakstīšanai. Cita pieeja ir ļaut modelēšanas metodei pašai konstruēt tādas bāzes funkcijas, kas ir nepieciešamas adekvātas paredzēšanas spējas regresijas modeļa izveidošanai. To ir iespējams veikt izmantojot tā saucamo bāzes funkciju konstruēšanas pieeju (Basis Function Construction, BFC). Izmantojot BFC, lietotājam nav jāizvēlas modeļa maksimālā pakāpe (vai jādefinē bāzes funkciju kopa). BFC automātiski konstruē nepieciešamās bāzes funkcijas, pielietojot heiristisku pārmeklēšanu, efektīvi atrodot kompromisu starp modeļa vienkāršību un paredzēšanas spēju. Rakstā praktiskā stiklšķiedras stieņa stabilitātes metamodelēšanas problēmā tiek salīdzinātas četras dažādas polinomu regresijas modelēšanas metodes: vienkāršā p-tās kārtas polinomu regresija, uz priekšu vērsta izvēle ar statistisko mēru F, uz priekšu vērstā izvēle ar AICC, kā arī BFC pieejas instance. Rezultāti uzrāda BFC pieejas pārākumu.

Jekabsons G., Kalnins K., Eglitis E. Polynomials in metamodeling of glass fibre bar stability

Typically, in metamodeling a low-order polynomial model is used – usually a second-order polynomial. However it cannot model highly nonlinear behaviours. Higher-order polynomials can be used, but instabilities may arise. As a possible remedy for the problem, subset selection techniques may be used. However they assume that the chosen fixed full set of predefined basis functions contains a subset which is sufficient to describe the target relation sufficiently well. Another approach is to let the modelling method itself construct the basis functions necessary for creating the regression model with adequate predictive performance. This can be done using the so-called Basis Function Construction approach (BFC). With BFC the user does not need to choose the maximal order of the models (or predefine the set of basis functions). BFC automatically constructs the necessary basis functions using heuristic search, efficiently trading-off the simplicity and predictive performance of the models. In the paper, in a practical glass fibre bar stability metamodeling problem, we compare four different polynomial regression modelling methods: a simple p-th order polynomial regression, Forward Selection with F-statistic, Forward Selection with AICC, as well as an instance of the BFC approach. The results show superiority of BFC approach.

Екабсон Г., Калныньш К., Эглитис Е. Полиномы в метамоделировании устойчивости стекловолоконных стержней

В метамоделировании, как правило, используется полином низкой степени – обычно полином второй степени. Однако, такой подход не обеспечивает моделирование поведения процессов с большей степенью нелинейности. Применение полиномов более высокой степени приводит к неустойчивости апркосиманта. Для решения этой проблемы можно использовать методы выбора подмножеств. Однако, при этом обычно предполагается, что определенное множество заранее выбранных базисных функций содержит подмножество функций, которые с достаточной степенью достоверности описывают процесс. Другой возможный подход предполагает конструирование подмножества функций самим методом моделирования. Подход реализует конструирование базисных функций (Basis Function Construction, BFC). Применяя BFC, пользователю нет необходимости выбирать максимальную степень модели (или определять множество базисных функций). BFC автоматически отыскивает необходимые базисные функции, применяя эвристические методы просмотра пространства положений, эффективно выбирая компромисс между простотой модели и способностью предвидения модели. В статье, на примере метамоделирования устойчивости стекловолоконного стержня, сравниваются четыре метода моделирования полиномиальной регрессии: простая полиномиальная регрессия степени p, вперед направленная выборка со статистической мерой F, вперед направленная выборка с критерием AICC и BFC подход. Результаты показывают преимущбество BFC подхода.