International Journal of Engineering & Technology, 7 (3.5) (2018) 32-36

International Journal of Engineering & Technology

Website: www.sciencepubco.com/index.php/IJET

Research paper

Experience in Using Stochastic Optimization Methods for Determining Numerical Parameters of Models in Materials Structurization Management Systems

Korneev Andrey Mastislavovich, Buzina Olga Petrovna, Sukhanov Andrey Vladimirovich, Shipulin Ilya Andreevich

[1]*Affiliation of the first author*
[2]*Affiliation of the second author*
[3]*Affiliation of the third author*
**Corresponding author E-mail: d.48@rambler.ru*

Abstract

The task of intellectual support of the process of composition formation for materials with a composite structure occurs when designing and operating automated control systems for multi-stage production processes. Such automated systems function in direct interaction with the external environment, and should promptly return the results of processing to the environment in the form of corrective actions or as messages to the user. The need for correct and complete mathematical models and fast, accurate algorithms that solve multistage problems often arises when structuring composite materials. In this case, mathematical models contain sets of numerical parameters and the search for exact values for them presents a complex optimization problem. The purpose of this paper is to investigate the possibility of using stochastic optimization methods to determine the exact numerical values of the calculated parameters of mathematical models that mimic the behavior of a structured composite material with given physico-mechanical characteristics under operating conditions. To carry out the research, special software has been created that implements algorithms for searching for extreme values for functions of several variables. The functional purpose of the software is intellectual support for decision-making in the formation of chemical compositions of cast iron alloys. Another developed system is designed to make effective decisions when designing the composition and structure of composite materials containing discrete fibers. Optimization of the calculated parameters was performed on a definite and fixed search area, which is a hyperparallelepiped. The program implements ten modifications of the simulation algorithm for annealing, allowing for a finite number of steps to make an estimate of the optimal value of the input elements of the function under study on a multidimensional space. In particular, modification of A, B and B algorithm schemes using the Boltzmann and Cauchy distribution functions, as well as the superfast annealing algorithm and the Xin Yao algorithm are implemented. The obtained data allowed to draw conclusions about the advantages and disadvantages of each modification of the stochastic search algorithm..

Keywords: *Optimization, Random value, Normal distribution, Stochastic search, Simulation method for annealing*

1. Introduction

To solve optimization problems are being developed numerous methods for stochastic search based on Markov processes [1, 2, 3]. In particular, one of the most effective methods for the case of optimizing multivariate objective function are metaheuristic: genetic algorithms, tabu search, simulated annealing, max-min ant system, ant colony optimization, particle swarm optimization, the method of differential evolution, etc. [4, 5. , 6]. Modern researchers recognized metaheuristics powerful and extremely popular class of optimization techniques that allow high efficiency to find solutions for a wide range of applications from different application [7, 8, 9, 10]. The advantage of metaheuristic methods based on stochastic algorithms lies in their ability to solve complex challenges in the absence of knowledge of the search space; moreover, a good implementation of the meta-heuristic method can ensure finding a solution close to optimal within a reasonable time or number of iterations. In many ways, this is why such methods allow us to find optimal solutions for problems that are difficult to solve from the point of view of direct analytical research. Very simplistic metaheuristics can be viewed as algorithms that implement a direct random search on a discrete space of possible optimal or near-optimal solutions of the problem until the conditions imposed or reached a predetermined number of iterations will be performed. The purpose of this paper is to investigate the possibility of using stochastic optimization methods to determine the exact numerical values of the calculated parameters of mathematical models that mimic the behavior of a structured composite material with given physico-mechanical characteristics under operating conditions.

2. Research Method

To carry out research, a computer program has been written that allows intellectual support for decision-making when forming the chemical composition of castings from cast iron. One of the modules of the program allows you to estimate the dependence of the speed of the stochastic search algorithm on its numerical input parameters, the initial temperature (T_0), the number of cycles (L) and the temperature decrease parameter (c). The main window of

the program is shown in Figure 1. A modification of the stochastic search algorithm is selected in a separate module.

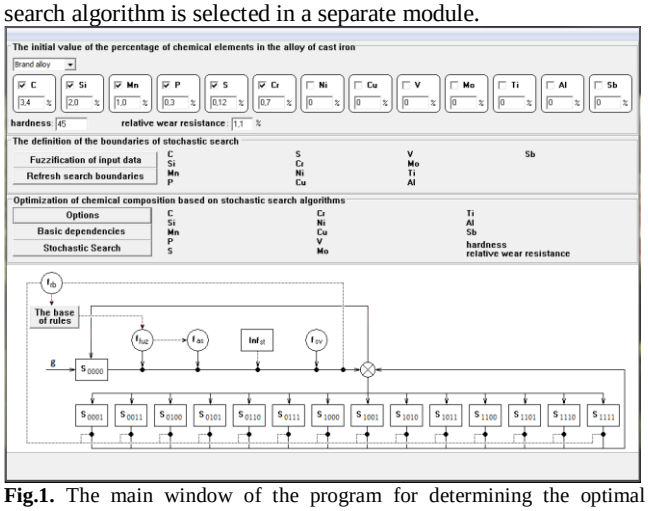

Fig.1. The main window of the program for determining the optimal chemical composition

Separately, software has been developed to make effective decisions when designing the composition and structure of composite materials containing discrete fibers. The system also allows you to predict the properties of the final product, - bent elements from the formed material. Managing the process of structuring and improving the quality of composite materials of complex structure is difficult because of the lack of uniform physical models that would allow both to identify the links between the quality criteria and the final properties, and to predict the reliability of the products. The complication of the processes affecting the stress-strain state of the elements, as well as the growth in the number of factors that determine the final properties of new materials, leads to an increase in the amount of experimental research needed to develop optimal modes of modeling and estimating the reliability of elements. Optimized parameters in equations describing the stress-strain state of elements are assisted by modified stochastic search algorithms on multidimensional spaces. The criterion of optimality here is the minimization of the difference in the values of full-scale tests and the results of computer calculations. The schemes of such algorithms are constructed taking into account the structure of the element, the modeling of which will be based on the diagram technique using the optimized values of the coefficients in the equations of approximation of the characteristic diagrams.

Stochastic optimization by annealing allows us to search for a finite number of steps in the global minimum (maximum) of some function $f(x)$ defined on some continuous or discrete space S. The values of the function f at points that are elements of the set S are represented as the energy of an imaginary physical system $E = f(x)$. The temperature of the system T, set at each moment, decreases with time. Each new state of the system is given in accordance with a given function $J(x, T)$, which is the generating family of probability distributions. The function $J(x, T)$ defines a random element $G(x, T)$ with values in the space S for fixed x and T. With probability equal to $h(\Delta E, T)$, the system after generating a new state $x' = G(x, T)$ goes to the next step (already in the state x'), otherwise the process of generating the state x' is repeated. Here $\Delta E = f(x') - f(x)$ is the increment of the energy function of the system, and the value of $h(\Delta E, T)$ is the probability of accepting a new state [3].

As a function specifying the probability of accepting a new state, either the exact value is chosen:

$$h(\Delta E, T) = \frac{1}{1 + \exp\left(\frac{\Delta E}{T}\right)}$$

either an approximate value

$$h(\Delta E, T) = \exp\left(-\frac{\Delta E}{T}\right)$$

The second formula is most often used [3].

The simplest version of the algorithm for the stochastic search method simulated annealing is:

1) The initial point $x = x_0$, $x_0 \in S$ is chosen randomly. The current value of the energy function of the system $E = f(x_0)$ is determined.

2) While the search stopping condition $T(k) < T_{end}$ is not fulfilled, perform the following steps of the k-th iteration of the main loop:

(a) Compare the values of the function E in the state x and in a state that is at the current moment a global minimum. If the value of $E = f(x)$ is smaller, then change the global minimum value.

(b) Generate a new state $x' = G(x, T)$.

(c) Determine the value of the function in the new state $E' = f(x')$.

(d) Generate a random number $\alpha \in [0, 1]$.

(e) If $\alpha < p(\Delta E, T(k))$, set $x \leftarrow x'$, $E \leftarrow E'$ and go to iterations of k+1. If $\alpha \geq p(\Delta E, T(k))$ repeat step (b) until an appropriate point x 'is found.

The following modifications of the above algorithm are possible:

Modification A. In step 2e, if the point x' is not suitable, a transition to the next iteration is possible provided that the next iteration starts at x with a new value of the decreasing parameter T.

Modification B. For the case of large dimension S, in order to accelerate the operation of the algorithm, the last value of x is taken as an estimate of the global minimum point. However, this approach can lead to a worse solution, especially if the value of the parameter T significantly exceeds zero by the time the algorithm finishes.

Modification B. At the beginning of the algorithm, step x 1 assumes $x \leftarrow x_0$, and in step 2b a new point x' is calculated recursively by the formula $x' = G(x', T)$. This approach allows the algorithm to "not get stuck". However, with such an implementation, the simulated annealing algorithm is practically no different from the usual stochastic search, which leads to the loss of a number of advantages of the algorithm.

One of the most common schemes of the simulated annealing method is the Boltzmann scheme (Boltzmann annealing). In this scheme, the change in the parameter T of the algorithm is given by the formula:

$$T(k) = \frac{T_0}{\ln(1+k)}, \quad k > 0.$$

The density of probability distributions is chosen as a family of normal distributions with mathematical expectation x and variance T:

$$g(x'; x, T) = \frac{1}{(2\pi T)^{D/2}} \cdot \exp\left(-\frac{|x' - x|^2}{2T}\right),$$

where D is the dimension of the metric state space. The main drawback of this scheme is the slow decrease in temperature T. For this reason, the researchers of Hartley and Tsu [11] proposed an algorithm scheme in which the formula T

$$T(k) = \frac{T_0}{k}.$$

Under this scheme, there is no loss of guarantee of finding the minimum due to the use of the normalized Cauchy distributions with density

$$g(x';x,T)=\frac{1}{\pi^{(D+1)/2}}\cdot\frac{T}{\left(|x'-x|^2+T^2\right)^{(D+1)/2}}.$$

In this scheme, the global minimum is determined to be guaranteed only when the parameter T changes with a speed not exceeding

$$T(k)=\frac{T}{k^{1/D}},$$

which is much slower than the Boltzmann scheme [3].

In order to eliminate the shortcomings of the two described methods, L. Ingber proposed the method of ultrafast fast search (Very Fast Annealing) [11, 12]. In the proposed scheme, the space S is considered to consist of vectors of dimension D:

$$\begin{pmatrix}x_1\\ \mathrm{M}\\ x_n\end{pmatrix},\ x_i\in[A_i,B_i].$$

For each of the coordinates, the parameter *T* can be different, i.e. *T* is also a vector in a space of dimension *D*. The family of distributions is constructed as follows. The value $y = \Delta x/(B_i - A_i)$ is introduced; The new search value x 'is calculated by the formula

$$x_i'=x_i+z_i(B_i-A_i)$$

where z_i is a random variable on the set [-1, 1] with the distribution density

$$g_T(y)=\prod_{i=1}^{D}\frac{1}{2(|y_i|+T_i)\ln\left(1+\frac{1}{T_i}\right)}\equiv\prod_{i=1}^{D}g_{(i,T)}(y_i),$$

$$y_i\in[-1,1].$$

The random variable zi is modeled as follows:

$$z_i=\mathrm{sgn}\left(\alpha_i-\frac{1}{2}\right)\cdot T_i\left(\left(1+\frac{1}{T_i}\right)^{|2\alpha_i-1|}-1\right),$$

where αi are independent random variables uniformly distributed on the interval [0; 1].

The advantage of the superfast search scheme is that it allows a very rapid simulation of the distribution densities G, regardless of the dimensionality of the set S.

Another method of ultrafast search is the algorithm proposed by Xin Yao [11, 12]. The uniqueness of the method lies in the repeated application of the scheme of the previous algorithm. The distribution density is given here by the following method:

$$g_T(y)=\prod_{i=1}^{D}g_{(i,T)}(y_i)=\prod_{i=1}^{D}\frac{1}{2\left(|y_i|+\frac{1}{\ln(1/T_i)}\right)\ln\left(1+\ln(1/T_i)\right)}.$$

3. Results and Analysis

In the general case, the behavior of the system under investigation is described by the following laws of functioning $f:R^d\to R^{2n}$.

1) When optimizing the parameters {Ξ} = {ξ1, ..., ξ48}:

$$\begin{pmatrix}M_{x1} & \dots & M_{xn}\\ f_{x1} & \dots & f_{xn}\end{pmatrix}=f\left(\{\mathrm{H}\},\{\mathrm{E}\},\{\Delta\},\{W_{S0i},P_{S0i}\},\{W_{H0i},P_{H0i}\},\{\Xi\}\right),$$

where f_{xi} is the deflection in the central section of the disperse object with respect to the X axis; Mxi is the bending moment with respect to the X axis; {H} = { *h* is the cross sectional height, *b* is the section width, l_f is the length of the discrete fiber, d_f is the diameter of the section of the discrete fiber} - geometric characteristics of the elements of the disperse object; {E} = {R_b, R_{bt}, R_f} - strength characteristics of the elements of the disperse object; {Δ} = {E_b, E_f, ε_{bR}, ε_{btR}, ε_{fbtR}} - deformation characteristics; {W_{S0i}, P_{S0i}}, {W_{H0i}, P_{H0i}} are the coordinates of the characteristic piecewise linear diagrams of the displacements of a single discrete fiber in the matrix of the disperse object; *n* is the number of results of the computational experiment.

2) When optimizing the parameters { $\overline{\Xi}$ } = { $\overline{\xi}_1$, ..., $\overline{\xi}_9$ }:

$$\begin{pmatrix}M_{x1} & \dots & M_{xn}\\ f_{x1} & \dots & f_{xn}\end{pmatrix}=f\left(\{\mathrm{H}\},\{\mathrm{E}\},\{\Delta\},\{\Phi\},\{W_{S0i},P_{S0i}\},\{W_{H0i},P_{H0i}\},\{\Xi\},\{\overline{\Xi}\}\right),$$

where {Φ} = {$r_{cp,j}$ are the averaged distances between discrete fibers; $k_{A,j}$ - coefficients that take into account the contact interaction between discrete fibers; φ_j - angles of orientation of discrete fibers} - characteristics of the location and orientation of discrete fibers in the matrix of a dispersed object.

3) When optimizing the parameters { $\widetilde{\Xi}$ } = { $\widetilde{\xi}_1$, ..., $\widetilde{\xi}_3$ }:

$$\begin{pmatrix}M_{x1} & \dots & M_{xn}\\ f_{x1} & \dots & f_{xn}\end{pmatrix}=f\left(\{\mathrm{H}\},\{\mathrm{E}\},\{\Delta\},\{\Phi\},\{W_{S0i},P_{S0i}\},\{W_{H0i},P_{H0i}\},\{\Xi\},\{\overline{\Xi}\},\{\widetilde{\Xi}\}\right)$$

The objective function of finding the global minimum is:

$$\sum_{i=1}^{n}\left|M_{xi}-M_{xi}^{ex}\right|+\sum_{i=1}^{n}\left|f_{xi}-f_{xi}^{ex}\right|\to 0,$$

where M_{xi}^{ex} and f_{xi}^{ex} are the experimental values of the bending moment and deflection, respectively.

Since, when optimizing the parameters, the values of M_{xi} will be compared for fixed values of f_{xi}, then

$$\sum_{i=1}^{n}\left|f_{xi}-f_{xi}^{ex}\right|=0,$$

the target function will be minimized by the values of M_{xi}:

$$\sum_{i=1}^{n}\left|M_{xi}-M_{xi}^{ex}\right|\to 0$$

Values

$$\begin{pmatrix}M_{x1} & \dots & M_{xn}\\ f_{x1} & \dots & f_{xn}\end{pmatrix}$$

are determined by the calculation of the nonlinear-deformation model on the basis of individual algorithms.

The search areas for each of the coefficients ξ_1, …, ξ_{48} are presented in Table 1.

Table 1. Areas of search for optimal values of sets Ξ, $\overline{\Xi}$, $\widetilde{\Xi}$

Coefficient	Search scop	Coefficient	Search scop	Coefficient	Search scop	Coefficient	Search scop

	e		e		e		e
ξ_1	[-1; 1]	ξ_{16}	[0; 10]	ξ_{31}	[0; 10]	ξ_{46}	[0; 200]
ξ_2	[-1; 1]	ξ_{17}	[-2; 1]	ξ_{32}	[0; 10]	ξ_{47}	[0; 10]
ξ_3	[-1; 1]	ξ_{18}	[-2; 1]	ξ_{33}	[-1; 10]	ξ_{48}	[0; 10]
ξ_4	[-1; 1]	ξ_{19}	[-1; 1]	ξ_{34}	[-1; 10]	$\bar{\xi}_1$	[0; 2]
ξ_5	[0; 300]	ξ_{20}	[-1; 1]	ξ_{35}	[-3; 3]	$\bar{\xi}_2$	[0; 1]
ξ_6	[0; 10]	ξ_{21}	[0; 500]	ξ_{36}	[-3; 3]	$\bar{\xi}_3$	[0; 30]
ξ_7	[0; 300]	ξ_{22}	[0; 100]	ξ_{37}	[0; 300]	$\bar{\xi}_4$	[0; 10]
ξ_8	[0; 10]	ξ_{23}	[0; 10]	ξ_{38}	[0; 300]	$\bar{\xi}_5$	[0; 10]
ξ_9	[-1; 1]	ξ_{24}	[0; 10]	ξ_{39}	[0; 10]	$\bar{\xi}_6$	[-10; 10]
ξ_{10}	[-1; 1]	ξ_{25}	[-1; 5]	ξ_{40}	[0; 10]	$\bar{\xi}_7$	[0; 10]
ξ_{11}	[-1; 1]	ξ_{26}	[-1; 5]	ξ_{41}	[-1; 15]	$\bar{\xi}_8$	[-10; 10]
ξ_{12}	[-1; 1]	ξ_{27}	[-2; 2]	ξ_{42}	[-1; 15]	$\bar{\xi}_9$	[1; 30]
ξ_{13}	[0; 200]	ξ_{28}	[-2; 2]	ξ_{43}	[-4; 4]	$\tilde{\xi}_1$	[0; 2]
ξ_{14}	[0; 10]	ξ_{29}	[0; 400]	ξ_{44}	[-4; 4]	$\tilde{\xi}_2$	[0; 1]
ξ_{15}	[0; 200]	ξ_{30}	[0; 400]	ξ_{45}	[0; 200]	$\tilde{\xi}_3$	[0; 10]

In the random search algorithm for simulated annealing of optimal parameters Ξ by the Boltzmann scheme, it was customary to modify the Gibbs distribution function. The Gibbs distribution function here has the form:

$$P(\Delta E, T_k) = \begin{cases} 1, & \Delta E < 0, \\ \exp\left(-\dfrac{\Delta E}{T_k} \cdot I_{\text{mod}}\right), & \Delta E \geq 0. \end{cases},$$

where I_{mod} is the modification coefficient, defined by the formula:

$$I_{\text{mod}} = \left| 1 - \sqrt[n]{\prod_{j=1}^{n} \left| \frac{M'_{xj}}{M^{e}_{xj}} \right|^{1/j}} \right|.$$

This factor takes into account the accumulation of deviations of the values of M_{xj} from the values of the full-scale experiment M^{e}_{xj}. The function E goes to the new state of the system E' with a higher probability in the case that the values M_{xj} and M^{e}_{xj} is approach. Here, we take into account the decrease in the degree of influence of the points ξ_i for i>24 on the search result, namely, the last coordinates of the diagram «f_x-M_x» depend on these points, the values of which «accumulate» the errors in the calculation of the nonlinear deformation mathematical model on the basis of the deterministic algorithm.

In Figure 2. graphically represents the approximation of the points ξ_{29}, ξ_{30} (every hundredth iteration) to the found optimal value. When searching, the modeled Boltzmann scheme of modification A was used based on the algorithm shown in Fig. 3.2. In the algorithm, the following values of the parameters T are accepted: T_0 = 50, T_{end} = 3,5; the number of steps of the search algorithm is 1600320.

In Fig. 3. A similar approximation of points to the optimal value is presented using the Boltzmann scheme of modification B.

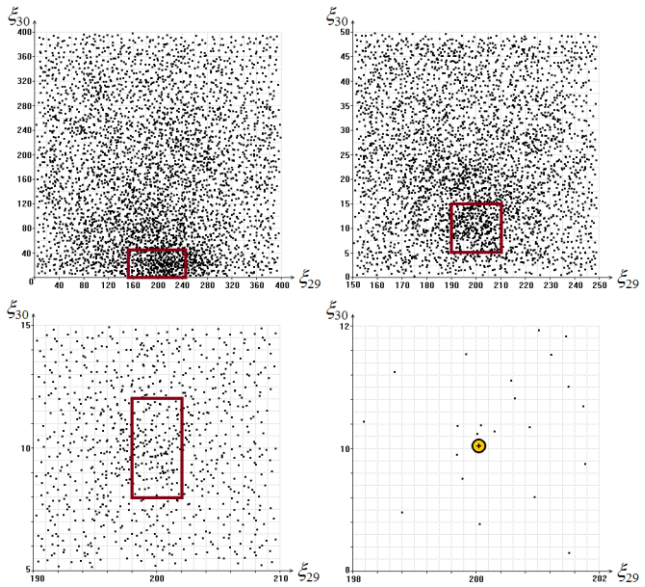

Fig. 2. Approximation of the values of the parameters ξ_{29}, ξ_{30} to the optimal values in the process of stochastic search in the Boltzmann scheme (modification A)

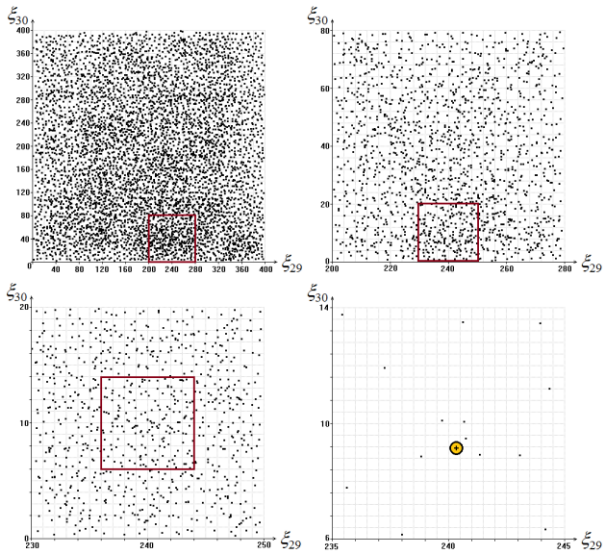

Fig. 3. Approximation of the values of the parameters ξ_{29}, ξ_{30} to the optimal values in the process of stochastic search in the Boltzmann scheme (modification B)

4. Conclusion

From the results of computational experiments it is clear that the algorithms for ultrafast annealing and Xin Yao have the greatest accuracy in determining the extremal values of functions of several variables. The results obtained using algorithms based on Boltzmann and Cauchy schemes have deviations from optimal (maximum) values. At the same time, the rate of convergence of the Xin Yao algorithm substantially exceeds the rate of convergence of other algorithms. An essential advantage of the ultrafast annealing algorithm and the Xin Yao algorithm and modification B of the algorithm based on the Boltzmann scheme is a small dispersion of the results of the optimization of the function, i.e. The search for the optimal value using these algorithms will not lead to significant errors in repeated use. Note that for modified algorithms based on the Boltzmann and Cauchy schemes, it is possible to correct the calculated parameters-the maximum (initial) temperature, the number of cycles, the temperature decrease parameter, in such a way that the accuracy of the calculation results increases with increasing time and, conversely, not requiring high accuracy of the results obtained, to achieve the speed of calcula-

tions. Thus, algorithms based on the annealing simulation method are the most suitable for applied research, since it allows variants of the relationship between the accuracy of calculations and the rate of convergence of stochastic search.

Since each search pattern produces different results, the optimality of which is not guaranteed with a 100% result, several modifications of the circuits need to be considered. The computer model makes it possible to estimate the closeness of the stochastic coefficient values obtained from the characteristic diagrams to the optimal ones by comparing the data of the computational experiment carried out using the obtained values of the coefficients to the data of the full-scale experiment. Thus, it is possible to select from several results for various schemes of stochastic search those whose use of the results will create the most adequate simulation model for describing the stress-strain state of a dispersed object with discrete fibers. To this end, the following modifications of the Boltzmann scheme of stochastic search were modeled.

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