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INVESTIGATION AND COMPARISON OF ITERATION CURVES OF OPTIMIZATION ALGORITHMS

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Abstract: The iteration history curve of optimization algorithms is a saturation- type development curve or sigmoid shape curve. After an overview of several different sigmoid curves, the iteration history curve of the RVA (Random Virus Algorithm) is analysed in order to find its best settings for a given optimization problem. The analysis of the characteristics and numerical parameters of the iteration history curve provides the possibility to discover the speed and efficiency of the algorithm without the necessity to wait throughout the whole running until its final result, which can speed up numerical experiments during the search for the solution to the optimization problem and while 'fine tuning' the algorithm to the given task. Since sigmoid-type curves can be found in many different fields of life (the history of the sport world records, comparison of the achievements of several groups), the results of this analysis can be used in several different domains of life, when the ranking, comparison, evaluation or qualification of several individuals or groups is important.

Keywords: Iteration history curves, sigmoid curves, saturation curves, comparison of algorithms, group achievements.

1. INTRODUCTION

Each optimization algorithm has some very important numerical parameters which can have important effects on the behaviour and characteristics of the algorithm. These important characteristics could be the 'speed' (how many objective function evaluations are necessary until finding the final optimum solution), or the 'efficiency' (how many times the constraints are checked until finding the optimum solution). These characteristics are strongly connected with the quantity of the necessary calculations to be performed until the optimum result. These days Multidisciplinary Optimization (MDO) is a very common approach (Abraham, Hassanien, Siarry, & Engelbrecht, 2009), (Cramer, Dennis, Jr., Frank, Lewis, & Shubin, 1994), (Martins & Lambe, 2013), (Szabó, 2008), (Vanderplaats, 2007) and more and more structures are being analysed by MDO methods. During an MDO task, the evaluation of the objective function and/or the checking the constraints may require long finite element computations, therefore the computer running of these investigations could take even several days. Nowadays evolutionary optimization offers efficient algorithms for the solution of these tasks (Das, Dasgupta, Biswas, Abraham, & Konar, 2009), (Deb, 2007), (Eberhart & Kennedy, 1995), (Fogel, 1999.), (Gao, Hongwei, Zhao, & Cui, 2006), (Goldberg, 1989), (Martens, et al., 2007), (Sheel, 1985). Engineering Design Optimization is also an increasingly popular field in optimization science (Herskovits, Mappa, Goulart, & Mota Soares, 2005), (Pang, Chen, Wang, & Hou, 2012), (Zhang, Zhou, Zhou, Wang, & Zhang, 2005), (Szabó, 2016).

Because the parameters of the algorithm can have important effects on the most important characteristics of the algorithm, by modifying these parameters it may be possible to spare a significant amount of calculations, so we could decrease the number of days necessary for finding the final solution. The procedure for changing the settings of these parameters and finding the effects of these settings on the value of the optimum solution and on the time and calculation amount necessary to reach to goal, can be called 'numerical experiments' on the algorithm settings. If the total running time of the algorithm can be several days, this means we have to wait for several days in order to see the effects of the current settings of the algorithm parameters. After that there will be the time necessary to evaluate and understand these effects, and to determine some new values to improve the settings. Once more several days will be necessary to see the new results and find the effects of these new settings. This procedure makes the total time of the numerical experiments process very long.

In this paper the RVA optimization algorithm (Szabó, 2008) is used to demonstrate the usage and efficiency of the iteration curve analysis, showing the numerical experiment (parameter setting combinations) process for a simple optimization task. The analysis of the equations of the sigmoid curves can be used not only for investigating one algorithm, but for the comparison of several algorithms (for the same test problem for example), thus it could be possible to find the best algorithm for the given optimization problem.

Sigmoid curves describing growth or saturation phenomena are used in many fields of life for description, study and forecast of these kinds of situations. These curves are highly multidisciplinary curves, because one can find many different applications of these curves in a large variety of problems (biology – population dynamics,

economy – lifecycle curve of products, medicine – growth of tumours or time history of pandemic disease just like COVID 19, environmental protection – plastic waste in oceans, agriculture – growth of fishes and forests, optimization – iteration history curve of optimization algorithms).

Discovery and investigation of the sigmoid curves started in the years of 1700. Malthus (Malthus, 1798), who proved that the increase in the number of members of a species is dependent from the actual value of this number. This is the basis of the Moore (Moore, 1965) law for computers capacity increase. Verhulst (Verhulst, 1847) derived the sigmoid curve describing the case of saturation, introducing the denomination of this type of curve 'logistic curve' or logistic function. Pearl and Reed (Pearl & Reed, 1920) applied the logistic curve for the study of the population growth of USA. The S-like shape of the curve made possible to use the attribute "sigmoid" for these curves. Fisher and Pry (Fisher & Pry, 1971) developed a transformation of the curves from S-shape into linear function, which makes easier to calculate the regression coefficient in case of approximation of the curves. Bertalanffy (Von Bertalanffy, 1960) used sigmoid curves for the description of the growth of the length of sharks, these results are useful also for the study of several fish species and in forestry too. Kozuko and Bajzer (Kozuko & Bajzer, 2003) applied this growth function for the study of the growth of tumours in medicine. The growth function modified by Richards (Richards, 1959) is applicable for the studies of the growth of several plants, too.

Mansfield (Mansfield, 1961) and Rogers (Rogers, 1962) described the products lifecycle as sigmoid curve. Jang Show- Ling, Dai, and Sung (Jang, Dai, & Sung, 2005) shown that the spread of the mobile phones in 29 OECD countries and Taiwan can be described also by sigmoid curves. Investigating some pulsating or multi-wave phenomena by Meyer (Meyer & Turner II, 1994) shown the possibility of the application of bi-logistic, tri-logistic or multi-logistic curves, which were used by Silverberg and Lehnert (Silverberg & Lehnert, 2003) for the investigation of the evolutionary models of economic growth. Fokasz (Fokasz, 2006) gave interesting examples of the application of sigmoid curves for social phenomena.

Szabó investigated several phenomena by sigmoid curves: one hundred years history of sports world records (Szabó, 2011), proposed a comparison and qualification system using sigmoid curves (Szabó, 2017) having the name EBSYQ (Evolutionary Based System for Qualification and comparison of group achievements), investigated the iteration history curves of optimization algorithms (Szabó, 2018), studied the possible future of the plastic waste in oceans of the Earth (Szabó, 2019), investigated wear curves of tools (Szabó, 2021), shown that product lifecycle can be described also by sigmoid curves (Vajna, 2020), (Bihari & Sarka, 2018), investigated the time curve of COVID 19 disease in Hungary (Szabó, 2020). For all these

investigations Szabó applied the approximation procedure based on the Nelder-Mead optimization algorithm (Nelder & Mead, 1965), defined the approximation process as an optimization procedure searching for the minimum of the square differences. Rézsó (Rézsó, 2020) shown an example for the application of the EBSYQ system for the comparison of several student groups writing the same exam test. Because sigmoid type curves can be found in many different fields of the life (history of the sport world records, comparison of the achievements of several groups), the results of this kind of analysis can be used in several different domains of life; anywhere where the ranking, comparison, evaluation or qualification of several individuals or groups is important. This could help the work of teachers of student groups, jury members of grants and competitions, or selection teams and committees for job applications, adjudications of grants or awards, etc.

2. OVERVIEW OF SOME SIGMOID CURVES

The iteration history curve of the RVA optimization algorithm for a simple demonstration optimization problem can be found in Figure 1. It can be seen from the figure, that in the beginning phase of the optimization, the improvement in the objective function is high over several generations, but this 'improvement speed' decreases in the final phase of the optimum search. This effect can be called 'saturation', and this gives the sigmoid shape of the curve.

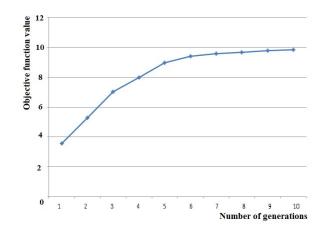


Figure 1. Iteration history curve of RVA algorithm

On the basis of the mathematical representation of the iteration history sigmoid curve of the algorithm, it will be possible to see the most important parameters determining the shape of the curve and also the most important characteristics of the result (maximum possible value achievable, steepness of the curve which is in connection with the improvement speed of objective function, etc.). If the curve is approximated by using only the first 3-4 iterations, it is not necessary to wait for the total running time of the algorithm; the current setting can be evaluated and qualified much earlier. This gives the possibility for developers to save more than the half of the total development time, which is an important achievement.

Table 1 shows the curve shape, the first derivative and the integral function shape of several different sigmoid type functions, in order to see and compare the most important characteristics of the sigmoid shape curves. One can draw some conclusions from the Table 1. Two different types of curves are possible: in the beginning phase with a curvature (e.g., Pearl-Reed function), or without beginning curvature (e.g., Bertalanffy function). Maybe it is not the curve itself that has the sigmoid shape but its integral (e.g., Life-curve). The derivative of the curves also can have different shapes (e.g., a Törnquist curve, Mitscherlich curve, Life-curve, or Pearl-Reed curve). For further investigations three curves will be selected: the Pearl-Reed curve because of its beginning curvature, one curve without beginning curvature (Bertalanffy), and later the Life-curve because of its very special shape.

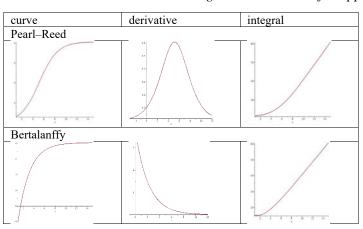


 Table 1

 Sigmoid curves used for approximation

Equations of the curves and their derivatives or integrals are as follows:

a.) Pearl-Reed (logistic) curve (Pearl & Reed, 1920): equation of the curve:

$$y(x) = \frac{K}{1 + ce^{-rx'}} \text{ first derivative: } \frac{dy(x)}{dx} = \frac{Kcre^{-rx}}{(1 + ce^{-rx})^2}$$
(1)

integral:
$$\int y(x)dx = -\frac{K}{r}\ln(e^{-rx}) + \frac{K}{r}\ln(1 + ce^{-rx})$$
 (2)

b.) Bertalanffy growth-curve (Von Bertalanffy, 1960): equation of the curve:

$$y(x) = K(1 - ce^{-rx})$$
, first derivative: $\frac{dy(x)}{dx} = Krce^{-rx}$ (3)

integral:
$$\int y(x)dx = Kx + \frac{Kc}{r}e^{-rx}$$
 (4)

Since the real iteration history curve of the studied algorithm can be either a growthcurve type, or a logistic curve, it is enough to select two curves (the Bertalanffy curve and the Pearl-Reed curve) from the six sigmoid curves of Table 1. Analysis of the Life-curve (equation of the curve, derivative, integral of it) may give further special results (eigenvalue of the algorithm, Lorentz-profile (Lorentz, 1905), spreading characteristics).

3. APPROXIMATION OF THE CURVES

The iteration history curve will be approximated by the Pearl-Reed and Bertalanffy curve, by using the method of least squares, determining the parameter values of K, r, c in the equation of the curves which give the best approximation to the iteration history curve.

During the method of least squares it is necessary to approach the given discrete values: (xi, yi), i = 1, 2, 3, ..., n, by a function $y^* = f(x)$, while the parameters of the curve should give the minimum possible value of the sum of the squares of the differences. This means that regarding the function values $f(xi) = y^*i$, we have to find:

$$H = \sum_{i=1}^{n} (y_i - y_i^*)^2 = min$$
(5)

The minimum is possible if the first derivative of the function H is 0, therefore: $\frac{\partial H}{\partial K} = 0$, $\frac{\partial H}{\partial r} = 0$, $\frac{\partial H}{\partial c} = 0$, this gives three equations for the three unknowns K, r and c, so it is possible to find the parameters for the best approximation. Another possible way to find the minimum of H as a function of the three parameters, is to solve the problem as an unconstrained minimization task of H using the three parameters as design variables. In this paper this method of optimization is selected for the

calculation of the best curve-parameters during the approximations. For the numerical solution of this optimization task the Nelder-Mead 'simplex' algorithm (Nelder & Mead, 1965) is used.

The linear regression coefficient will be used to check the quality of the approximation. Thus it is necessary to calculate the regression coefficient for both of the curves. Since the two selected curves are non-linear, before the analysis of the regression it is necessary to transform the equations of the curves into linear form. The regression coefficient calculated for these resulting linear functions will show which curve has the better correlation with the discrete data, so the conclusions derived from that curve will be stronger, or more realistic.

The value of the regression coefficient is always between -1 and +1. If it has a value of 0, that means there is no relationship between the curve and the discrete values. The closer the regression coefficient's absolute value to 1, the better the correlation is between the data and the approximation curve. If the regression coefficient is negative, it shows a decreasing tendency, while positive value shows an increase. This means that the conclusions derived from a curve having a 'weak' regression coefficient will be not 'true', not 'strong' or not accurate enough, but the conclusions derived on the basis of a curve having good correlation will be true and adequate, or 'strong'.

For calculation of the regression coefficient, the curve equations need to be transformed into linear form for both of the selected functions. The linear transformation of the Bertalanffy- function:

$$y(x) = K(1 - ce^{-rx}), ce^{-rx} = \frac{K - y(x)}{K}, \ln c + \ln e^{-rx} = \ln\left(\frac{K - y(x)}{K}\right),$$
(6)

therefore, linear function for the Bertalanffy -curve is: $y^* = a + bx$, where $a = \ln c$, b = -r.

The linear transformation of the Pearl-Reed function can be done in a similar way:

$$y(x) = \frac{K}{1 + ce^{-rx}}, \frac{K - y(x)}{y(x)} = ce^{-rx}, \ln c + \ln e^{-rx} = \ln \frac{K - y(x)}{y(x)}, y^* = a + bx$$
(7)

The regression coefficient can be calculated as:

$$R_{lin} = \frac{A_{xy} - \frac{B_{xy}}{n}}{\sqrt{\left(C_x - \frac{D_x}{n}\right)\left(C_y - \frac{D_y}{n}\right)}}$$
(8)

where: $A_{xy} = \sum_{i=1}^{n} x_i y_i$, $B_{xy} = \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i$, $C_x = \sum_{i=1}^{n} x_i^2$, $D_x = (\sum_{i=1}^{n} x_i)^2$ and $C_y = \sum_{i=1}^{n} y_i^2$, $D_y = (\sum_{i=1}^{n} y_i)^2$.

In equation (8) it is possible to calculate the linear regression coefficient of the y^* transformed function determined in equation (6) or (7), but for simplicity we return to the y notation.

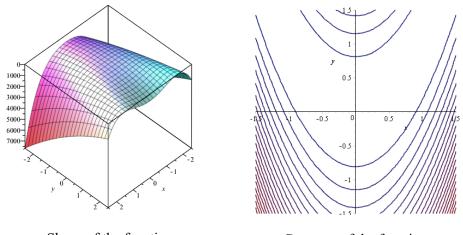
4. DEMONSTRATION EXAMPLE

In order to show the steps of the numerical experiments, let us consider the following simple optimization problem: Find the maximum of the two variables Rosenbrock-function (9) (Rosenbrock, 1960):

$$f(x, y) = 10 - (1 - x)^2 - 100(y - x^2)^2$$
(9)
cit constraints are:

when the explicit constraints are:

 $-2.5 \le x \le 2.5$ and $-2.5 \le y \le 2.5$, implicit constraint: $x^2 + y^2 \le 2$. The shape and contours of the objectives function are shown in Figure 2.



Shape of the function Contours of the function

Figure 2. The objective function of the optimization example

The solution of the problem is that the maximum of the f(x, y) is 10 at x = 1 and y = 1.

For the solution the RVA (Random Virus Algorithm) optimization algorithm is used and the iteration history curve of the algorithm is shown in Figure 1. This curve is a sigmoid function having saturation behaviour; therefore the Pearl-Reed function and the Bertalanffy-function is used for its approximation. The approximation of the iteration history curve can be seen in Figure 3 which shows that all the three curves (the original curve, the Pearl-Reed curve and the Bertalanffy curve) are very close each to another, so any of the selected two curves can be used for the approximation.

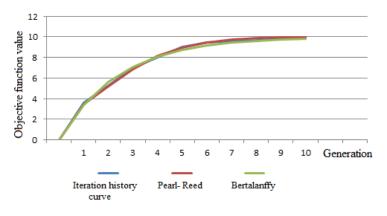


Figure 3. Approximation of the original iteration history curve

For further investigations the Bertalanffy curve seems to be better to use, because in the original iteration history curve the initial curvature of the Pearl-Reed curve is missing, therefore the shape of the curve is closer to the Bertalanffy curve. Also the regression coefficient absolute value is higher for the Bertalanffy curve than for the Pearl-Reed curve. However, because of the very special shape of its derivative, the Pearl-Reed function could give some interesting additional information during comparisons of several algorithms.

Equations of the approximating curves:

Pearl-Reed curve: $y = \frac{K}{1+ce^{-rx}}$, K = 10, r = 0.7, c = 3.8, regression coefficient value: -0.99183.

Bertalanffy curve: $y = K(1 - ce^{-rx})$, K = 10, r = 0.41, c = 1, regression coefficient: -0.99607.

The curves of the approximating functions can be seen in Figure 4 and their derivatives in Figure 5.

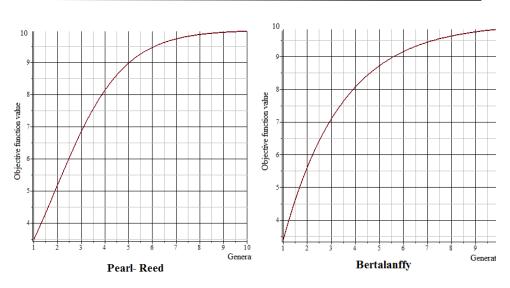


Figure 4. The approximating functions

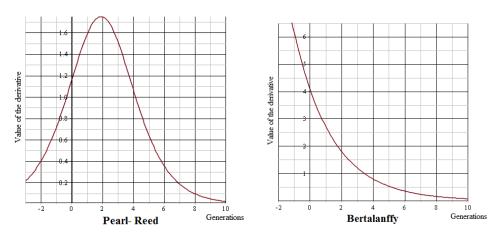


Figure 5. First derivative of the approximating functions

The derivative functions show the speed of the increasing of the objective function. It can be seen in Figure 5 that this speed decreases at higher number of iterations. The derivative of the Pearl-Reed function can say more: it shows, where the maximum of this speed is. This could be useful information if we want to compare several

algorithms, because a better algorithm should have this maximum earlier, since this will give a more efficient search in the starting phase of the optimization. The width of the Pearl-Reed derivative curve in the half of its maximum shows how durable this maximum speed is, so it could be also very useful for the comparisons of several optimization algorithms.

The integral function of the approximating curves is presented in Figure 6.

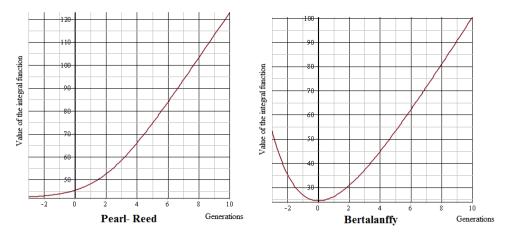


Figure 6. Integral of approximation curves

Comparison of the integral function of the approximating Pearl-Reed and Bertalanffy curves of the iteration history curve shows that the beginning phase of the search is more efficient for the Pearl-Reed function than for the Bertalanffy curve (because the same number of iterations shows a higher value of the integral function). In case of a higher number of iterations (or in the final phase of the optimization) the integral functions are parallel, so in this phase there is no difference in the efficiency. These curves can be very useful during the comparison of several algorithms.

In Figure 5 the first derivative of the Pearl-Reed function shows that the most efficient part of the optimization is the first phase of the process, with four generations, since the speed increase of the best objective function value of the generations is highest here. This leads to the idea to use only the first four iterations for building up the approximation curves of the iteration history curve, in this way saving 60% of the total time. There is no need to wait until the end of the total running time of the algorithm, we can guess the expectable optimum result. On the basis of this result, it is possible to change the settings of the algorithm and continue the numerical experiment. This method will decrease the total development time by more than 50%. Comparing the curves belonging to different settings of the algorithm parameters, it is possible to compare different states of the algorithm and will be easier to find the best setting values. Therefore, by using the proposed system of comparison the numerical experiment process can be made quicker and more accurate, based on the numerical comparison of different characteristics of the iteration history curves resulting from the settings.

Since the shape of the Life function and the derivative of the Pearl-Reed function (logistic function) is very similar, it seems to be useful to approximate the derivative of the logistic function with the equation of the Life-curve (Lorentz, 1905), (Andrews, 1998), because this way it will be possible to study the dispersion function (derivative of the Life-curve) and the error-function (integral of the Life-curve) of the algorithm, too (Figure 7.).

Here K = 1.73, r = 1.85, c = 0.32. The regression coefficient is 0.98381.

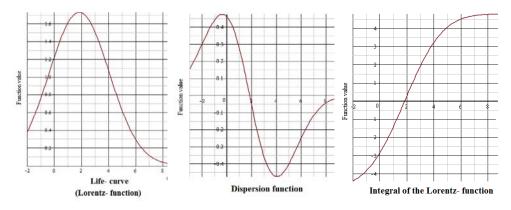


Figure 7. Life-curve, dispersion function and error function of the algorithm

Equation of the approximating Life-curve of the algorithm (the Lorentz-function):

$$f(x) = \frac{K}{e^{c^2(x-r)^2}}$$
(10)

The dispersion function is the derivative of the Life-curve:

$$f'(x) = -\frac{K(2c^2x - 2c^2r)}{e^{c^2(x-r)^2}}$$
(11)

The integral of the Life-curve is the error function of the algorithm:

$$\int f(x) dx = \frac{K\sqrt{\pi}}{2c} \operatorname{erf} \left(c(x-r) \right), \text{ where } \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$
(12)

The error function of the algorithm is once more a sigmoid curve; therefore it could be also used for the comparison of different algorithms or to compare the different settings of the same algorithm. Smaller K in this function means smaller expectable value of the error function, so it seems to be better than higher K values. If r is smaller, the error function is not so steep, which could be better than higher r values (when the increase in the error function is slower).

Table 2

Short description of the point of view	Score of setting I	Score of setting II	Point of view winner
Expectable optimum (K), Pearl - Reed, (PR)	10	10	both
Expectable optimum (K), Bertalanffy, (Bfy)	10	10	both
Obj. function value increasing speed (r), PR	0.7	0.67	setting I
Obj. function value increasing speed (r), Bfy	0.41	0.39	setting I
Regression coefficient, PR	-0.99183	-0.98743	setting I
Regression coefficient, Bfy	-0.99607	-0.98832	setting I
Place of the speed maximum, PR derivative	2	3	setting I
Durability of the speed maximum, PR derivative	5	5	both
Algorithm efficiency from integral of PR	130	125	setting I
Algorithm efficiency from integral of Bfy	90	85	setting I
Eigenvalue in Life-curve	2	3	setting I
Durability in Life-curve	5	5	both
Error function K	1.73	1.75	setting I
Error function r	1.85	2.3	setting I
Maximum amplitude of the dispersion function	0.94	0.9	setting II
Half width of the dispersion function	8	7.8	setting II
Maximum expectable value of the error function K	4.85	5.25	setting I
Increasing speed of the error function r	0.592	0.678	setting I
Number of points of view won	16	6	setting I

Comparison of two different settings of the RVA algorithm

In Table 2 several points of view are collected comparing two different settings of the RVA algorithm for the demonstration example shown above. Comparing the two settings of the RVA optimization algorithm to the same problem, it can be concluded that the 'winning' setting will result the quicker and more efficient work of the algorithm. Applying the four-point approximation method for the sigmoid curve of the algorithm makes possible to decrease the total time necessary for the whole development process approximately by 50% comparing to the case when always waiting through the total running time of the algorithm with a given setting.

Results and comparison points of view presented in this work are parts of the EB-SYQ (Evolution Based System for Qualification of Group Achievements) curve analysis system (Szabó, 2017), which is a comparison and evaluation system developed for the qualification and evaluation of groups. It is intended to help the decision-making work of teachers of student groups and jury of competitions, grants, or awards, but it is based also on sigmoid curves and one can find or 'translate' more useful comparison points of view from that system into the algorithm comparison process, too.

Main steps of the usage of the EBSYQ system: set up the points of view (which represent the most important characteristics to be compared), see the curves and equations for comparing these points of view, and compare how many points of view has won each item (group, algorithm, or setting) to be compared.

Table 3

Comparing setting parameters of the curve obtained by four points and of the curve obtained by waiting through the total running time (original curve)

	К	r	c
Original curve	10	0.41	1.0
Four points curve	9.88	0.39	0.97

According to the results shown in Table 2, Setting I is the winner, winning 73% of the total possible points. Taking only the four first generations of the iteration history, the Bertalanffy curve of the algorithm was approximated with the parameters shown in Table 3. It can be seen that the values are in good agreement, which means that by using this evaluation system, it is possible to cut down the total development time by more than half, during the numerical experiments process.

5. SUMMARY

The iteration history curve of optimization algorithms is a sigmoid shape saturation curve. The parameters in the equations of these curves are strongly connected to the most important characteristics of the algorithm (best objective function value increasing speed in function of the number of generations, expectable final optimum result, etc.). These characteristics can be efficiently modified by the setting parameters of the optimization algorithm. A complete numerical experiment process is needed for finding the best setting constellation for a given optimization problem. In

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order to see the effects of the settings, normally it is necessary to wait until the algorithm has finished running, which can be very long in case of some complicated Multidisciplinary Optimization problems. This paper shows a proposed approximation and analysis system of the algorithm's iteration curve (EBSYQ) which makes possible to set up the iteration curve's equation from just the objective function best values of the first four generations. This gives the possibility to reduce the total time needed for the numerical experiment process by more than 50%.

During these investigations it is very interesting to discover the Lorentz-curve, the eigenvalue and dispersion function of the algorithm, which can give important additional information about the characteristics and behaviour of the investigated algorithm. The integral of the Lorentz-function is the error function (erf) of the algorithm, while the parameters of this curve also give very useful points of view for describing and characterizing the algorithm's speed and efficiency. On the basis of these results, it is possible to investigate one algorithm with several different setting constellations or to compare several different algorithms for the same optimization task in order to find the most efficient or quick one.

In this paper the example of the RVA algorithm is shown applied for the optimization of the Rosenbrock-function over a cylindrical feasible region in order to demonstrate the steps, the usage and efficiency of the EBSYQ curve analysis system. Two different setting constellations are compared and using 18 points of view the better setting can be selected for the optimization task. Continuing the setting change and comparing process, it is possible to find the settings that give the quickest or most efficient working of the algorithm.

The results and points of view of the EBSYQ system can be used for the analysis of several other problems in real life, such as selection and comparison of different groups applying for grants, for scholarships or for jobs (jury activity) or for sport results analysis during a time period, while teachers of several student groups can discover more accurately different sub-groups of their students and they can find more easily some target-groups for differentiated training or extra activities.

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