

Knowledge discovery from data: InterCriteria Analysis of mutation rate influence

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Abstract: In this paper the InterCriteria Analysis (ICrA) approach is applied to find more knowledge from series of identification procedures using 34 differently tuned genetic algorithms (GAs). The influence of the mutation rate p_m on the algorithm performance is investigated. An *E. coli* fed-batch fermentation process model is used as a test problem. Based on the results from parameter identification, namely objective function values, the GAs, with the correspondent p_m -value, producing the best results are determined. Further, ICrA is applied using information from all model parameter estimates, computational time and objective function value. The ICrA confirms the conclusions based only on objective function values and helps to choose what mutation rate p_m is more appropriate to use in the considered case study.

Keywords: InterCriteria analysis, Intuitionistic fuzzy sets, Genetic algorithms, Mutation rate, *E. coli*.

2010 Mathematics Subject Classification: 03E72.

1 Introduction

InterCriteria Analysis (ICrA), proposed by [4], is a recently developed approach for evaluation of multiple objects against multiple criteria and thus discovering existing correlations between the criteria themselves. Various applications of the ICrA approach have been found in science

and practice – neural networks [19], properties of the crude oils [20], e-learning [11], algorithms performance [8], ecology [10], etc.

The ICrA is applied for establishing certain relations, considering parameters identification of cultivation models applying genetic algorithms (GAs). GA is a stochastic global optimization method. Among a number of optimization techniques, GA is one of the methods based on biological evolution and inspired by Darwin's theory of survival of the fittest [9].

In [17] the investigation is particularly focused on the relations between the *E. coli* cultivation model parameters μ_{max} , k_S and $Y_{X/S}$, on one hand, and the GA parameter *ggap* (generation gap), the convergence time and the model accuracy, on the other hand. Authors in [1] searched for relations between six *S. cerevisiae* cultivation model parameters, GA parameter population size, and GA outcomes – convergence time and objective function value. The results show that, based on ICrA, additional useful knowledge about identification procedures of cultivation process models can be derived and better performance of genetic algorithms can be achieved. Moreover, such research leads to a deeper understanding of the relations between the cultivation process model parameters.

Following these results, another important GA parameter, namely mutation rate p_m , is investigated here. The choice of mutation rate is one of the critical issues to the success performance of genetic algorithms [14, 15]. In this research the focus is on the influence of p_m on the model accuracy (value of the optimization criterion J), convergence time T and model parameters estimations. Thus, differently tuned GAs (with different p_m values) could be compared and some conclusions about the most appropriate mutation rate could be done.

An *E. coli* fed-batch fermentation model is considered as a case study. This process has been chosen as a representative of some of the important microorganisms with numerous applications in food and pharmaceutical industry, as well as one of the widely used model organisms in genetic engineering and cell biology, due to their well known metabolic pathways [13].

The paper is organized as follows: the problem formulation is given in Section 2, while Section 3 presents the background of ICrA. Numerical results and discussion are presented in Section 4 and conclusion remarks are given in Section 5.

2 Investigation on mutation rate influence

The mathematical model of the *E. coli* fed-batch fermentation process is presented by the following non-linear differential equations system [6]:

$$\frac{dX}{dt} = \mu_{max} \frac{S}{k_S + S} X - \frac{F_{in}}{V} X \quad (1)$$

$$\frac{dS}{dt} = -\frac{1}{Y_{S/X}} \mu_{max} \frac{S}{k_S + S} X + \frac{F_{in}}{V} (S_{in} - S) \quad (2)$$

$$\frac{dV}{dt} = F_{in} \quad (3)$$

where X is the biomass concentration, [g/l]; S is the substrate concentration, [g/l]; F_{in} is the feeding rate, [l/h]; V is the bioreactor volume, [l]; S_{in} is the substrate concentration in the feeding

solution, [g/l]; μ_{max} is the maximum value of the μ , [1/h]; k_S is the saturation constant, [g/l]; $Y_{S/X}$ is the yield coefficient, [-].

The following parameter vector $p = [\mu_{max} \ k_S \ Y_{S/X}]$ (see Eqs. (1)-(3)) should be identified using GAs with different values of mutation rate.

Model parameters identification is performed based on real experimental data for biomass and glucose concentration. The detailed description of the process conditions and the experimental data is given in [18].

The impact of p_m will be examined by choosing 34 different values of this genetic parameter. The chosen values of p_m are as follows:

$$p_m = [0.001, 0.004, 0.007, 0.01, 0.013, 0.016, 0.019, 0.022, 0.025, 0.028, 0.031, \\ 0.034, 0.037, 0.04, 0.043, 0.046, 0.049, 0.052, 0.055, 0.058, 0.061, 0.064, \\ 0.067, 0.07, 0.073, 0.076, 0.079, 0.082, 0.085, 0.088, 0.091, 0.094, 0.097, 0.1]. \quad (4)$$

The interval of p_m values from 0.001 to 0.1 is chosen on the basis of the reported results [7, 12, 16]. While the mutation rate is varied using vector p_m , all the other parameters and operators are kept constant (see Table 1) and thus 34 differently tuned GAs are constructed.

Table 1: Main GA parameters and operators

Parameters and operators	Values
number of individuals	100
number of generations	100
crossover rate	0.7
mutation rate	p_m
generation gap	0.97
crossover operator	double point
mutation operator	bit inversion
selection operator	roulette wheel selection
encoding	binary

With so constructed GAs, series of identification procedures of the mathematical model Eqs. (1)–(3) will be performed with the following objective function:

$$J = \sum_{i=1}^m (X_{\text{exp}}(i) - X_{\text{mod}}(i))^2 + \sum_{i=1}^n (S_{\text{exp}}(i) - S_{\text{mod}}(i))^2 \rightarrow \min \quad (5)$$

where m and n are the experimental data dimensions; X_{exp} and S_{exp} are the available experimental data for biomass and substrate; X_{mod} and S_{mod} are the model predictions for biomass and substrate with a given model parameter vector, $p = [\mu_{max} \ k_S \ Y_{S/X}]$.

3 InterCriteria analysis

Following [4] and [2], an Intuitionistic Fuzzy Pair (IFP), as the degrees of “agreement” and “disagreement” between two criteria applied on different objects, will be obtained. As a remainder, an IFP is an ordered pair of real non-negative numbers $\langle a, b \rangle$, such that $a + b \leq 1$.

For clarity, let an IM [3], whose index sets consist of the names of the criteria (for rows) and objects (for columns), be given. The elements of this IM are further supposed to be real numbers, which is not required in the general case. An IM with index sets, consisting of the names of the criteria, and IFPs, corresponding to the “agreement” and “disagreement” of the respective criteria, as elements will be obtained.

Let O denotes the set of all objects being evaluated, and $C(O)$ is the set of values assigned by a given criteria C (i.e., $C = C_p$ for some fixed p) to the objects, i.e.,

$$O \stackrel{\text{def}}{=} \{O_1, O_2, O_3, \dots, O_n\}, \quad C(O) \stackrel{\text{def}}{=} \{C(O_1), C(O_2), C(O_3), \dots, C(O_n)\}.$$

Let $x_i = C(O_i)$. Then the following set can be defined:

$$C^*(O) \stackrel{\text{def}}{=} \{\langle x_i, x_j \rangle | i \neq j \ \& \ \langle x_i, x_j \rangle \in C(O) \times C(O)\}.$$

Further, if $x = C(O_i)$ and $y = C(O_j)$, $x \prec y$ will be written iff $i < j$. The vectors of all internal comparisons for each criterion are constructed in order to find the agreement of different criteria. The elements of the vectors fulfil one of the three relations R , \bar{R} and \tilde{R} :

$$\langle x, y \rangle \in R \Leftrightarrow \langle y, x \rangle \in \bar{R}, \quad (6)$$

$$\langle x, y \rangle \in \tilde{R} \Leftrightarrow \langle x, y \rangle \notin (R \cup \bar{R}), \quad (7)$$

$$R \cup \bar{R} \cup \tilde{R} = C^*(O). \quad (8)$$

For example, if “ R ” is the relation “ $<$ ”, then \bar{R} is the relation “ $>$ ”, and vice versa. Hence, for the effective calculation of the vector of internal comparisons, denoted further by $V(C)$, only the subset of $C(O) \times C(O)$ needs to be considered, namely:

$$C^{\prec}(O) \stackrel{\text{def}}{=} \{\langle x, y \rangle | x \prec y \ \& \ \langle x, y \rangle \in C(O) \times C(O)\},$$

due to Eqs. (6)-(8). For brevity, $c^{i,j} = \langle C(O_i), C(O_j) \rangle$. Then, the vector with lexicographically ordered pairs as elements is constructed for a fixed criterion C :

$$V(C) = \{c^{1,2}, c^{1,3}, \dots, c^{1,n}, c^{2,3}, c^{2,4}, \dots, c^{2,n}, c^{3,4}, \dots, c^{3,n}, \dots, c^{n-1,n}\}. \quad (9)$$

Further, the vector $V(C)$ is replaced with $\hat{V}(C)$, where for the k -th component, $1 \leq k \leq \frac{n(n-1)}{2}$, it is true:

$$\hat{V}_k(C) = \begin{cases} 1 & \text{iff } V_k(C) \in R, \\ -1 & \text{iff } V_k(C) \in \bar{R}, \\ 0 & \text{otherwise.} \end{cases}$$

Then, the degree of “agreement” between two criteria, which are to be compared, is determined

as the number of the matching components, divided by the length of the vector for the purpose of normalization. This can be done in several ways, e.g. by counting the matches or by taking the complement of the Hamming distance. The degree of “disagreement” is the number of the components of opposing signs in the two vectors, again normalized by the length. This also may be done in various ways.

4 Numerical results and discussion

4.1 Parameter identification

The constructed 34 GAs are used to perform series of parameter identification procedures of the mathematical model (1)-(3). 30 independent runs have been performed for each GA in order to obtain reliable results for the total computation time, the objective function value and the model parameters estimations.

The obtained results of the 30 runs, for example in the cases of GA with $p_m = 0.001$ and GA with $p_m = 0.1$, have the following form:

$$GA_{0.001} = \begin{array}{c|ccccc} & \text{run1} & \text{run2} & \dots & \text{run29} & \text{run30} \\ \hline J & 4.7151729 & 4.7489781 & \dots & 4.6218317 & 4.6497095 \\ T & 63.9375 & 61.265625 & \dots & 61.40625 & 61.421875 \\ \mu_{max} & 0.5143830 & 0.5139544 & \dots & 0.5027635 & 0.5027634 \\ k_S & 0.01682812 & 0.0168291 & \dots & 0.0150506 & 0.0150455 \\ Y_{S/X} & 2.0212473 & 2.0223384 & \dots & 2.0225842 & 2.0225842 \end{array} \quad (10)$$

$$GA_{0.1} = \begin{array}{c|ccccc} & \text{run1} & \text{run2} & \dots & \text{run29} & \text{run30} \\ \hline J & 4.5832109 & 4.5281103 & \dots & 4.4571010 & 4.4604151 \\ T & 62.796875 & 62.484375 & \dots & 62.125000 & 62.203125 \\ \mu_{max} & 0.4993485 & 0.4940985 & \dots & 0.4845398 & 0.4845902 \\ k_S & 0.0143098 & 0.0131654 & \dots & 0.0112460 & 0.0113865 \\ Y_{S/X} & 2.0221000 & 2.0212442 & \dots & 2.0209313 & 2.0205553 \end{array} \quad (11)$$

The 34 IMs for all suggested p_m -values (see expression 4) are constructed in this manner. The full set of identification results is available at <http://intercriteria.net/studies/gap/mutr/>, because of the limited space here.

The obtained average values of the objective function for each GA, respectively each chosen values of p_m , are presented in Fig. 1. As can be seen, the p_m -value lower than 0.028 and greather than 0.073 do not produce good results. Two local minima – 4.48 and 4.49, are selected as the best estimates. Nine results for these two local minima are observed, marked in red circles in Fig. 1. The corresponding mutation rates p_m are listed in Table 2.

Table 2: Best J values

J value	4.48	4.49	4.49	4.49	4.49	4.48	4.49	4.49	4.49
p_m value	0.028	0.034	0.040	0.055	0.058	0.064	0.067	0.070	0.073

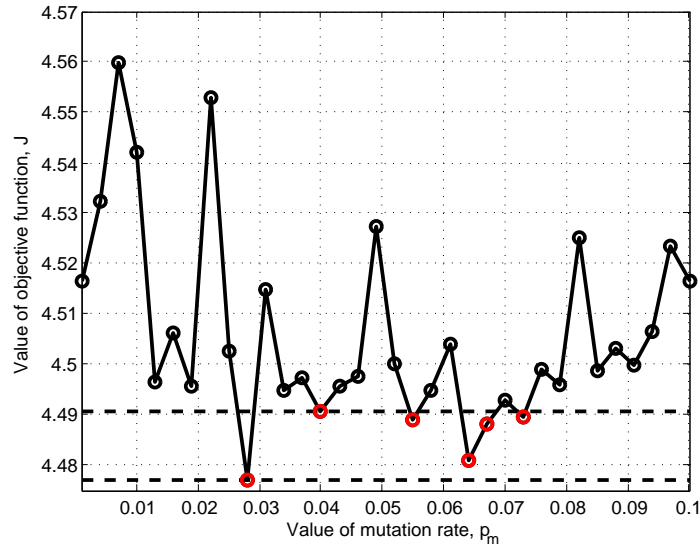


Figure 1: Obtained average values of J

The appropriate p_m -values for parameter identification of an *E. coli* fed-batch fermentation process, considered in this case study, are those listed in Table 2. In order to draw more conclusions about the influence of the mutation rate on GA performance, based on the obtained results, the ICRA is further applied. Thus, the overall GA performance is evaluated, based not only on the obtained J values, but on the basis of the total computational time T and the three model parameters estimates too.

4.2 ICRA of parameter identification results

The ICRA is performed to compare the performance of the 34 differently tuned GAs. All the 34 IMs (IM (10), IM (11) and the rest IMs in <http://intercriteria.net/studies/mutr/e-coli/results.zip>) are evaluated based on the ICRA algorithm. Thus, the degree of “agreement” ($\mu_{C,C'}$ -values) between GA outcomes, e.g. computation time (T), objective function value (J) and model parameters estimations (μ_{max} , k_S and $Y_{S/X}$) are evaluated. The resulting IM is presented by the Exp. (12), where the criterion $C1$ is the objective value J , $C2$ is the computation time T , $C3$ is the model parameter μ_{max} , $C4$ is the model parameter k_S and $C5$ is the model parameter $Y_{S/X}$.

For thus constructed IM (Exp. (12)), ICRA is applied again. The 34 different GAs are assumed as criteria and the 10 pairs of criteria are assumed as objects. As a result, 561 pairs of criteria are obtained. Intuitionistic fuzzy triangle representation is presented in the Fig. 2. Fig. 3 shows all observed $\mu_{C,C'}$ - and $\nu_{C,C'}$ -values, sorted in descending order of the $\mu_{C,C'}$ -values. Due to the large number of pairs, 561 criteria pairs, only some of them are printed in x-axis legend.

The scheme proposed in [5] is used (see Table 3) for analyses of the observed degree of “agreement” (consonance) and degree of “disagreement” (dissonance) between each pair of criteria.

Based on the scale presented in Table 3, 342 criteria pairs are found to be in positive consonance – 3 pairs in SPC, 89 in PC and 250 in WPC. The rest 219 criteria pairs are in dissonance. There are no pairs in negative consonance. Only the pairs that are in strong positive consonance

	$C1 - C2$	$C1 - C3$	$C1 - C4$	$C1 - C5$	$C2 - C3$	$C2 - C4$	$C2 - C5$	$C3 - C4$	$C3 - C5$	$C4 - C5$
$GA_{0.001}$	0, 531034	0, 590805	0, 475862	0, 579310	0, 639080	0, 494253	0, 643678	0, 648276	0, 733333	0, 604598
$GA_{0.004}$	0, 489655	0, 664368	0, 687356	0, 675862	0, 478161	0, 464368	0, 540230	0, 862069	0, 583908	0, 505747
$GA_{0.007}$	0, 489655	0, 797701	0, 790805	0, 390805	0, 501149	0, 496552	0, 462069	0, 956322	0, 257471	0, 236782
$GA_{0.01}$	0, 420690	0, 806897	0, 829885	0, 360920	0, 390805	0, 400000	0, 565517	0, 954023	0, 227586	0, 236782
$GA_{0.013}$	0, 602299	0, 655172	0, 675862	0, 632184	0, 480460	0, 533333	0, 547126	0, 845977	0, 498851	0, 491954
$GA_{0.016}$	0, 485057	0, 710345	0, 694253	0, 691954	0, 535632	0, 547126	0, 496552	0, 905747	0, 475862	0, 473563
$GA_{0.019}$	0, 595402	0, 498851	0, 487356	0, 728736	0, 485057	0, 450575	0, 544828	0, 827586	0, 471264	0, 377011
$GA_{0.022}$	0, 498851	0, 772414	0, 742529	0, 666667	0, 450575	0, 482759	0, 448276	0, 937931	0, 572414	0, 51954
$GA_{0.025}$	0, 549425	0, 827586	0, 777011	0, 616092	0, 537931	0, 540230	0, 508046	0, 917241	0, 475862	0, 406897
$GA_{0.028}$	0, 496552	0, 588506	0, 574713	0, 779310	0, 535632	0, 519540	0, 441379	0, 843678	0, 537931	0, 455172
$GA_{0.031}$	0, 494253	0, 774713	0, 712644	0, 595402	0, 478161	0, 480460	0, 616092	0, 864368	0, 471264	0, 372414
$GA_{0.034}$	0, 496552	0, 673563	0, 574713	0, 737931	0, 498851	0, 439080	0, 609195	0, 827586	0, 540230	0, 418391
$GA_{0.037}$	0, 632184	0, 691954	0, 627586	0, 698851	0, 581609	0, 526437	0, 613793	0, 880460	0, 510345	0, 418391
$GA_{0.04}$	0, 542529	0, 613793	0, 579310	0, 701149	0, 556322	0, 570115	0, 443678	0, 910345	0, 471264	0, 413793
$GA_{0.043}$	0, 491954	0, 547126	0, 496552	0, 733333	0, 471264	0, 360920	0, 570115	0, 834483	0, 501149	0, 367816
$GA_{0.046}$	0, 567816	0, 698851	0, 632184	0, 724138	0, 570115	0, 581609	0, 464368	0, 896552	0, 514943	0, 43908
$GA_{0.049}$	0, 466667	0, 754023	0, 731034	0, 611494	0, 427586	0, 400000	0, 475862	0, 871264	0, 498851	0, 416092
$GA_{0.052}$	0, 347126	0, 650575	0, 632184	0, 641379	0, 413793	0, 436782	0, 418391	0, 843678	0, 434483	0, 337931
$GA_{0.055}$	0, 487356	0, 691954	0, 650575	0, 747126	0, 434483	0, 443678	0, 489655	0, 944828	0, 549425	0, 512644
$GA_{0.058}$	0, 402299	0, 666667	0, 620690	0, 708046	0, 344828	0, 393103	0, 397701	0, 908046	0, 577011	0, 508046
$GA_{0.061}$	0, 570115	0, 671264	0, 593103	0, 691954	0, 494253	0, 519540	0, 466667	0, 760920	0, 597701	0, 404598
$GA_{0.064}$	0, 471264	0, 473563	0, 422989	0, 765517	0, 491954	0, 485057	0, 521839	0, 862069	0, 432184	0, 354023
$GA_{0.067}$	0, 409195	0, 586207	0, 540230	0, 698851	0, 508046	0, 514943	0, 402299	0, 866667	0, 579310	0, 505747
$GA_{0.07}$	0, 588506	0, 664368	0, 606897	0, 717241	0, 535632	0, 482759	0, 501149	0, 804598	0, 528736	0, 411494
$GA_{0.073}$	0, 526437	0, 560920	0, 528736	0, 728736	0, 314943	0, 370115	0, 512644	0, 802299	0, 547126	0, 404598
$GA_{0.076}$	0, 652874	0, 581609	0, 540230	0, 675862	0, 577011	0, 540230	0, 473563	0, 866667	0, 468966	0, 377011
$GA_{0.079}$	0, 620690	0, 549425	0, 494253	0, 779310	0, 519540	0, 531034	0, 537931	0, 848276	0, 567816	0, 489655
$GA_{0.082}$	0, 588506	0, 590805	0, 627586	0, 606897	0, 544828	0, 485057	0, 540230	0, 839080	0, 409195	0, 312644
$GA_{0.085}$	0, 496552	0, 563218	0, 505747	0, 836782	0, 480460	0, 494253	0, 487356	0, 887356	0, 487356	0, 411494
$GA_{0.088}$	0, 324138	0, 620690	0, 613793	0, 710345	0, 439080	0, 429885	0, 406897	0, 850575	0, 602299	0, 512644
$GA_{0.091}$	0, 485057	0, 565517	0, 586207	0, 611494	0, 487356	0, 496552	0, 482759	0, 910345	0, 462069	0, 464368
$GA_{0.094}$	0, 432184	0, 597701	0, 56092	0, 698851	0, 4942530	0, 471264	0, 459770	0, 880460	0, 540230	0, 457471
$GA_{0.097}$	0, 280460	0, 549425	0, 528736	0, 758621	0, 427586	0, 416092	0, 404598	0, 832184	0, 524138	0, 457471
$GA_{0.1}$	0, 577011	0, 629885	0, 583908	0, 797701	0, 698851	0, 675862	0, 491954	0, 898851	0, 519540	0, 473563

(12)

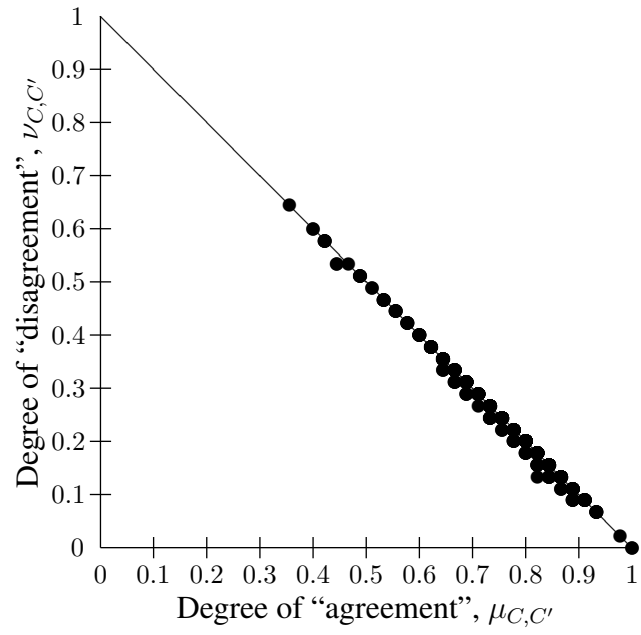


Figure 2: Intuitionistic fuzzy triangle representation

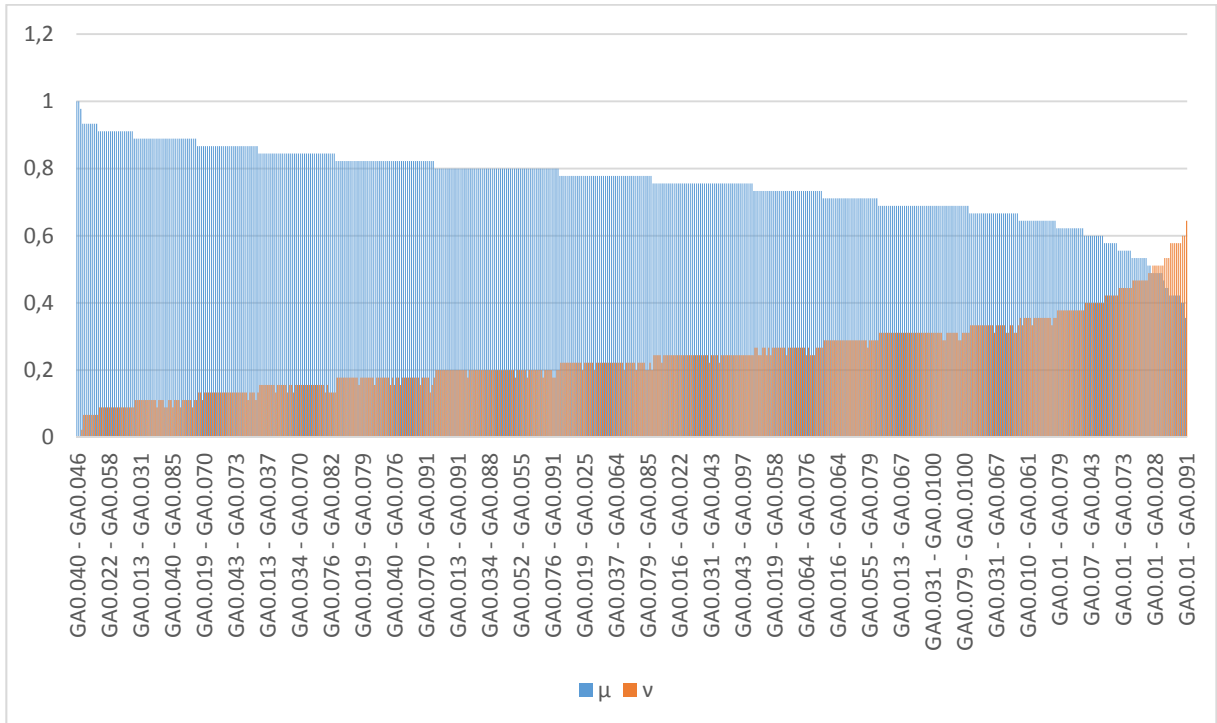


Figure 3: Sorted $\mu_{C,C'}$ - and $\nu_{C,C'}$ -values of the obtained 561 criteria pairs

Table 3: Consonance and dissonance scale

Interval of $\mu_{C,C'}$	Meaning
[0-0.05]	strong negative consonance (SNC)
(0.05-0.15]	negative consonance (NC)
(0.15-0.25]	weak negative consonance (WNC)
(0.25-0.33]	weak dissonance (WD)
(0.33-0.43]	dissonance (D)
(0.43-0.57]	strong dissonance (SD)
(0.57-0.67]	dissonance (D)
(0.67-0.75]	weak dissonance (WD)
(0.75-0.85]	weak positive consonance (WPC)
(0.85-0.95]	positive consonance (PC)
(0.95-1]	strong positive consonance (SPC)

(SPC) and in positive consonance (PC) are analysed further.

There are two criteria pairs that show the strongest degree of “agreement” ($\mu = 1$): $GA_{0.040} - GA_{0.046}$ and $GA_{0.088} - GA_{0.097}$. The value of $\mu = 0.97$ is observed only for one pair: $GA_{0.055} - GA_{0.058}$. For eight criteria pairs the value of $\mu = 0.93$ is obtained: $GA_{0.016} - GA_{0.025}$, $GA_{0.028} - GA_{0.067}$, $GA_{0.028} - GA_{0.094}$, $GA_{0.04} - GA_{0.091}$, $GA_{0.046} - GA_{0.091}$, $GA_{0.058} - GA_{0.073}$, $GA_{0.088} - GA_{0.094}$ and $GA_{0.094} - GA_{0.097}$.

Confirmation of the results presented in Table 2 is found in these results. According to ICRA, the best obtained results are in positive consonance, namely $GA_{0.055} - GA_{0.058}$, $GA_{0.028} - GA_{0.067}$, $GA_{0.058} - GA_{0.073}$. The strong relation between the pairs $GA_{0.055} - GA_{0.058}$ and $GA_{0.058} - GA_{0.073}$ suggests a strong relation between $GA_{0.055} - GA_{0.073}$, too. The ICRA results confirm this assumption – the degree of “agreement” μ for the pair $GA_{0.055} - GA_{0.073}$ is 0.91.

GA with $p_m = 0.04$ shows similar performance with $GA_{0.046}$ and $GA_{0.091}$, although these GAs obtain J -values greater than 0.49. This is due to the fact that ICRA takes into account all estimates ($T, \mu_{max}, k_S, Y_{S/X}$), not only the J -value.

For the rest three GAs listed in Table 2 is found that:

- GA with $p_m = 0.034$ shows some similar performance with GA with $p_m = 0.043$, respectively $\mu = 0.91$;
- GA with $p_m = 0.07$ shows higher degree of “agreement” in the following criteria pairs: $GA_{0.07} - GA_{0.037}$ and $GA_{0.07} - GA_{0.082}$, respectively $\mu = 0.91$; and $GA_{0.07} - GA_{0.04}$, $GA_{0.07} - GA_{0.046}$ and $GA_{0.07} - GA_{0.061}$, respectively $\mu = 0.9$;
- GA with $p_m = 0.064$ has not show similar performance with none of the others GAs. All pairs are found to be in dissonance.

5 Conclusion

Differently tuned GAs are investigated in this work in order to define the influence of the mutation rate p_m on the algorithm performance. 34 different values of p_m are used in the range between 0.001 and 0.1. The 34 GAs are applied to parameter identification of an *E. coli* fed-batch fermentation process model. Based on the obtained results, 9 GAs with following mutation rate p_m : 0.028, 0.034, 0.04, 0.055, 0.058, 0.067, 0.07 and 0.073, are defined as the best performed algorithms. Further, by applying ICrA, more knowledge about the identification results of all 34 GAs is sought. The algorithm performance in this case is evaluated based on data of all parameter estimates, computational time and objective function value. The obtained results confirm the previous choice of best performed GAs and gives an additional knowledge about the relation and correlation between the 34 investigated GAs.

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