

InterCriteria Analysis of a Model Parameters Identification using Genetic Algorithm

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Abstract—In this paper we apply an approach based on the apparatus of the Index Matrices and the Intuitionistic Fuzzy Sets – namely InterCriteria Analysis. The main idea is to use the InterCriteria Analysis to establish the existing relations and dependencies of defined parameters in non-linear model of an *E. coli* fed-batch cultivation process. Moreover, based on results of series of identification procedures we observe the mutual relations between model parameters and considered optimization techniques outcomes, such as execution time and objective function value. Based on InterCriteria Analysis we examine the obtained identification results and discuss the conclusions about existing relations and dependencies between defined, in terms of InterCriteria Analysis, criteria.

Index Terms—InterCriteria Analysis; Index matrices; Intuitionistic Fuzzy Sets; Genetic Algorithm; chromosomes; parameter identification; *E. coli*; fed-batch cultivation process.

I. INTRODUCTION

THE InterCriteria Analysis (ICA) is developed with the aim to gain additional insight into the nature of the criteria involved and discover on this basis existing relations between the criteria themselves [8]. It is based on the apparatus of the Index Matrices (IM) [10], [11], and the Intuitionistic Fuzzy Sets [12] and can be applied for decision making in different areas of science and practice. The approach has been discussed in a several papers [10], [14], [15], [16]. In [8] a possibility of the ICA method for criterion value prediction, proposing two algorithms, is presented. In [16] a discussion on the threshold values in the ICA was further elaborated. But, up to now, considering ICA application, the only applications reported are in one area: namely, EU member states competitiveness analysis [14], [15]. Encouraging results of these first applications of the ICA provoke us to use the method for establishing and identifying the relations between parameters of the mathematical model of an *E. coli* fed-batch cultivation process. The model parameters are further considered as criteria in terms of ICA.

In the case of modelling of cultivation processes ICA approach could be very useful. Cultivation processes are characterized with complex, non-linear dynamic and their modelling is a hard combinatorial optimization problem. On the one hand, the parameter identification is of key importance for modelling process and additional knowledge about the model parameters relations will be extremely useful to improve the model accuracy. On the other hand, the information may be used to improve the performance of the used optimization algorithms if, for instance, some algorithm outcomes are added to the considered criteria. Thus, the relations between model parameters and optimization algorithm performance will be established.

In this paper we applied the ICA to establish the basic relations between the parameters in the model of an *E. coli* fed-batch cultivation process. The existing relations are identified based on results of a series of parameters identification procedures. The use of meta-heuristic techniques such as Genetic Algorithms (GAs) has received more and more attention [3]. These methods offer good solutions, even global optima, within reasonable computing time [17], so we choose to use genetic algorithms for estimation of the model parameters.

The paper is organized as follows. The background of InterCriteria Analysis is given in Section 2. The problem formulation is described in Section 3. The numerical results and a discussion are presented in Section 4. Conclusion remarks are done in Section 5.

II. INTERCRITERIA ANALYSIS

Here we expand on the idea proposed in [8]. Following [8] and [12] we will obtain an Intuitionistic Fuzzy Pair (IFP) as the degrees of “agreement” and “disagreement” between two criteria applied on different objects. We remind briefly that an IFP is an ordered pair of real non-negative numbers $\langle a, b \rangle$ such that:

$$a + b \leq 1.$$

For clarity, let us be given an IM (see [10]) whose index sets consist of the names of the criteria (for rows) and objects (for columns). The elements of this IM are further supposed to be real numbers (in the general case, this is not required). We will obtain an IM with index sets consisting of the names of the criteria (for rows and for columns) with elements IFPs corresponding to the “agreement” and “disagreement” of the respective criteria.

Two things are further supposed (which are not always guaranteed in practice and, when not fulfilled, present an interesting direction for new research in themselves):

- 1) All criteria provide an evaluation for all objects (i.e. there are no inapplicable criteria for a given object) and all these evaluations are available (no missing evaluations).
- 2) All the evaluations of a given criteria can be compared amongst themselves.

Further by O we denote the set of all objects O_1, O_2, \dots, O_n being evaluated, and by $C(O)$ the set of values assigned by a given criteria C to the objects, i.e.

$$O \stackrel{\text{def}}{=} \{O_1, O_2, \dots, O_n\},$$

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

Let:

$$C^*(O) \stackrel{\text{def}}{=} \{\langle x, y \rangle \mid x \neq y \ \& \ \langle x, y \rangle \in C(O) \times C(O)\}.$$

In order to compare two criteria we must construct the vector of all internal comparisons of each criteria, which fulfill exactly one of three relations R , \bar{R} and \tilde{R} . In other words, we require that for a fixed criterion C and any ordered pair $\langle x, y \rangle \in C^*(O)$ it is true:

$$\langle x, y \rangle \in R \Leftrightarrow \langle y, x \rangle \in \bar{R}, \quad (1)$$

$$\langle x, y \rangle \in \tilde{R} \Leftrightarrow \langle x, y \rangle \notin (R \cup \bar{R}), \quad (2)$$

$$R \cup \bar{R} \cup \tilde{R} = C^*(O). \quad (3)$$

From the above it is seen that we need only consider a subset of $C(O) \times C(O)$ for the effective calculation of the vector of internal comparisons (denoted further by $V(C)$) since from (1), (2) and (3) it follows that if we know what is the relation between x and y we also know what is the relation between y and x . Thus we will only consider lexicographically ordered pairs $\langle x, y \rangle$. Let, for brevity:

$$C_{i,j} = \langle C(O_i), C(O_j) \rangle.$$

Then for a fixed criterion C we construct the vector:

$$V(C) = \{C_{1,2}, C_{1,3}, \dots, C_{1,n}, C_{2,3}, C_{2,4}, \dots, C_{2,n}, C_{3,4}, \dots, C_{3,n}, \dots, C_{n-1,n}\}.$$

It can be easily seen that it has exactly $\frac{n(n-1)}{2}$ elements. Further, to simplify our considerations, we replace the vector

$V(C)$ with $\hat{V}(C)$, where for each $1 \leq k \leq \frac{n(n-1)}{2}$ for the k -th component 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 when comparing two criteria we determine the “degree of agreement” between the two as the number of matching components (divided by the length of the vector for normalization purposes). 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 components of opposing signs in the two vectors (again normalized by the length). This also may be done in various ways. A pseudocode of the algorithm used in this study for calculating the degrees of agreement and disagreement between two criteria C and C' is presented below.

Algorithm 1 Calculating “agreement” and “disagreement” between two criteria

Require: Vectors $\hat{V}(C)$ and $\hat{V}(C')$

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1: function DEGREE OF AGREEMENT( $\hat{V}(C), \hat{V}(C')$ )
2:    $V \leftarrow \hat{V}(C) - \hat{V}(C')$ 
3:    $\mu_{C,C'} \leftarrow 0$ 
4:   for  $i \leftarrow 1$  to  $\frac{n(n-1)}{2}$  do
5:     if  $V_i = 0$  then
6:        $\mu_{C,C'} \leftarrow \mu_{C,C'} + 1$ 
7:     end if
8:   end for
9:    $\mu_{C,C'} \leftarrow \frac{2}{n(n-1)} \mu_{C,C'}$ 
10:  return  $\mu_{C,C'}$ 
11: end function

12: function DEGREE OF DISAGREEMENT( $\hat{V}(C), \hat{V}(C')$ )
13:   $V \leftarrow \hat{V}(C) - \hat{V}(C')$ 
14:   $\nu_{C,C'} \leftarrow 0$ 
15:  for  $i \leftarrow 1$  to  $\frac{n(n-1)}{2}$  do
16:    if  $\text{abs}(V_i) = 2$  then ▷ abs: absolute value
17:       $\nu_{C,C'} \leftarrow \nu_{C,C'} + 1$ 
18:    end if
19:  end for
20:   $\nu_{C,C'} \leftarrow \frac{2}{n(n-1)} \nu_{C,C'}$ 
21:  return  $\nu_{C,C'}$ 
22: end function

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It is obvious (from the way of calculation) that for $\mu_{C,C'}$, $\nu_{C,C'}$, we have:

$$\mu_{C,C'} = \mu_{C',C}, \nu_{C,C'} = \nu_{C',C}.$$

Also, $\langle \mu_{C,C'}, \nu_{C,C'} \rangle$ is an IFP.

III. PROBLEM FORMULATION

Let us use the following non-linear differential equation system to describe the *E. coli* fed-batch cultivation process [1], [4]:

$$\frac{dX}{dt} = \mu X - \frac{F_{in}}{V} X, \quad (4)$$

$$\frac{dS}{dt} = -q_S X + \frac{F_{in}}{V} (S_{in} - S), \quad (5)$$

$$\frac{dV}{dt} = F_{in}, \quad (6)$$

where

$$\mu = \mu_{max} \frac{S}{k_S + S}, \quad q_S = \frac{1}{Y_{S/X}} \mu \quad (7)$$

and 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 and q_S are the specific rate functions, [1/h]; 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, [-].

For the model (Eq. (4)-Eq. (7)) the parameters that will be identified are μ_{max} , k_S and $Y_{S/X}$.

Let $Z_{mod} \stackrel{\text{def}}{=} [X_{mod} \ S_{mod}]$ (model predictions for biomass and substrate) and $Z_{exp} \stackrel{\text{def}}{=} [X_{exp} \ S_{exp}]$ (known experimental data for biomass and substrate). Then putting $Z = Z_{mod} - Z_{exp}$, we define the objective function as:

$$J = \|Z\|^2 \rightarrow \min, \quad (8)$$

where $\|\cdot\|$ denotes the ℓ^2 -vector norm.

For the model parameters identification we use experimental data for biomass and glucose concentration of an *E. coli* MC4110 fed-batch fermentation process. The detailed description of the process condition and experimental data are presented in [2].

To estimate the model parameters we applied consistently 14 differently tuned GA. We use various population sizes – from 5 to 200 chromosomes in the population. The number of generations is fixed to 200. The main GA operators and parameters are summarized in Table I. Because of the stochastic nature of the applied algorithms we perform series of 30 runs for each population size. Thus, we obtain the average, best and worst estimate of the parameters, as well as of the algorithm execution time and value of objective function. The detailed description of identification procedure is given in [7].

To perform ICA three IMs are constructed – the IM A_1 (Eq. 9) with the obtained average results, the IM A_2 (Eq. 10) with the best obtained results and IM A_3 (Eq. 11) with the worst obtained results. In addition to the presented in [7] results here the average, worst and best estimates for the tree model parameters in all 14 cases are given too. Thus, five criteria are considered – C_1 is parameter μ_{max} , C_2 is parameter k_S , C_3 is parameter $Y_{S/X}$, C_4 is objective function value J and C_5 is resulting execution time T .

TABLE I
MAIN GA OPERATORS AND PARAMETERS

Operator	Type
fitness function	linear ranking
selection function	roulette wheel selection
crossover function	simple crossover
mutation function	binary mutation
reinsertion	fitness-based
Parameter	Value
generation gap	0.97
crossover probability	0.75
mutation probability	0.01
number of generations	200

IV. NUMERICAL RESULTS AND DISCUSSION

Computer specification to run all identification procedures are Intel Core i5-2329 3.0 GHz, 8 GB Memory, Windows 7 (64bit) operating system.

Based on the presented **Algorithm 1** the ICA is implemented in the Matlab 7.5 environment. We obtain IMs that determine the degrees of “agreement” ($\mu_{C,C'}$) and “disagreement” ($\nu_{C,C'}$) between criteria for the three cases.

1) *Case of average results:*

Resulting degrees of “agreement” ($\mu_{C,C'}$) are as follows:

	C_1	C_2	C_3	C_4	C_5	
$IM_1 =$	C_1	1	0.91	0.41	0.74	0.26
	C_2	0.91	1	0.36	0.78	0.27
	C_3	0.41	0.36	1	0.55	0.38
	C_4	0.74	0.78	0.55	1	0.11
	C_5	0.26	0.27	0.38	0.11	1

Resulting degrees of “disagreement” ($\nu_{C,C'}$) are as follows:

	C_1	C_2	C_3	C_4	C_5	
$IM_2 =$	C_1	0	0.08	0.58	0.26	0.74
	C_2	0.08	0	0.62	0.21	0.71
	C_3	0.58	0.62	0	0.44	0.60
	C_4	0.26	0.21	0.44	0	0.89
	C_5	0.74	0.71	0.60	0.89	0

2) *Case of worst results:*

Resulting degrees of “agreement” ($\mu_{C,C'}$) are as follows:

	C_1	C_2	C_3	C_4	C_5	
$IM_5 =$	C_1	1	0.79	0.34	0.88	0.14
	C_2	0.79	1	0.18	0.84	0.22
	C_3	0.34	0.18	1	0.33	0.64
	C_4	0.88	0.84	0.33	1	0.07
	C_5	0.14	0.22	0.64	0.07	1

Resulting degrees of “disagreement” ($\nu_{C,C'}$) are as follows:

$A_1(average) =$

	GA ₅	GA ₁₀	GA ₂₀	GA ₃₀	GA ₄₀	GA ₅₀	GA ₆₀	GA ₇₀	GA ₈₀	GA ₉₀	GA ₁₀₀	GA ₁₁₀	GA ₁₅₀	GA ₂₀₀
C_1	0.552	0.525	0.515	0.491	0.486	0.508	0.497	0.498	0.498	0.496	0.494	0.500	0.492	0.489
C_2	0.022	0.021	0.018	0.013	0.010	0.016	0.014	0.013	0.014	0.014	0.012	0.015	0.013	0.011
C_3	2.032	2.025	2.019	2.023	2.023	2.020	2.022	2.022	2.022	2.021	2.023	2.021	2.021	2.023
C_4	6.271	5.838	4.760	4.561	4.646	4.607	4.580	4.568	4.578	4.570	4.553	4.547	4.560	4.545
C_5	4.649	6.053	7.472	11.248	12.917	14.649	16.973	19.719	21.793	24.196	26.848	29.515	39.406	51.917

$A_2(best) =$

	GA ₅	GA ₁₀	GA ₂₀	GA ₃₀	GA ₄₀	GA ₅₀	GA ₆₀	GA ₇₀	GA ₈₀	GA ₉₀	GA ₁₀₀	GA ₁₁₀	GA ₁₅₀	GA ₂₀₀
C_1	0.491	0.480	0.494	0.491	0.488	0.492	0.488	0.490	0.484	0.491	0.488	0.486	0.488	0.488
C_2	0.013	0.011	0.013	0.012	0.012	0.012	0.012	0.013	0.011	0.013	0.012	0.012	0.012	0.012
C_3	2.023	2.024	2.018	2.023	2.020	2.023	2.020	2.019	2.019	2.020	2.019	2.021	2.019	2.018
C_4	4.833	4.855	4.475	4.482	4.444	4.449	4.463	4.438	4.447	4.450	4.425	4.433	4.458	4.436
C_5	4.867	5.912	7.675	11.295	13.229	15.007	17.316	20.062	22.667	24.757	26.926	30.015	39.780	52.323

$A_3(worst) =$

	GA ₅	GA ₁₀	GA ₂₀	GA ₃₀	GA ₄₀	GA ₅₀	GA ₆₀	GA ₇₀	GA ₈₀	GA ₉₀	GA ₁₀₀	GA ₁₁₀	GA ₁₅₀	GA ₂₀₀
C_1	0.577	0.538	0.544	0.518	0.521	0.517	0.515	0.510	0.510	0.505	0.489	0.510	0.504	0.511
C_2	0.015	0.026	0.024	0.018	0.019	0.018	0.018	0.016	0.017	0.015	0.012	0.016	0.015	0.016
C_3	2.037	1.995	2.019	2.021	2.021	2.021	2.020	2.022	2.021	2.022	2.022	2.023	2.022	2.022
C_4	9.296	9.618	5.363	5.009	4.967	4.864	4.808	4.736	4.746	4.721	4.702	4.732	4.672	4.721
C_5	5.600	5.632	7.301	10.827	12.496	14.399	16.801	19.500	21.715	23.915	27.051	29.188	39.921	51.309

TABLE II
CRITERIA RELATIONS SORTED BY $\mu_{C,C'}$ VALUES

$IM_6 =$

	C_1	C_2	C_3	C_4	C_5
C_1	0	0.20	0.65	0.12	0.86
C_2	0.20	0	0.80	0.15	0.77
C_3	0.65	0.80	0	0.66	0.35
C_4	0.12	0.15	0.66	0	0.93
C_5	0.86	0.77	0.35	0.93	0

3) Case of best results:

Resulting degrees of “agreement” ($\mu_{C,C'}$) are as follows:

$IM_3 =$

	C_1	C_2	C_3	C_4	C_5
C_1	1	0.74	0.49	0.63	0.36
C_2	0.74	1	0.35	0.53	0.51
C_3	0.49	0.35	1	0.71	0.30
C_4	0.63	0.53	0.71	1	0.25
C_5	0.36	0.51	0.30	0.25	1

Resulting degrees of “disagreement” ($\nu_{C,C'}$) are as follows:

$IM_4 =$

	C_1	C_2	C_3	C_4	C_5
C_1	0	0.19	0.44	0.33	0.59
C_2	0.19	0	0.59	0.44	0.46
C_3	0.44	0.59	0	0.26	0.68
C_4	0.33	0.44	0.26	0	0.75
C_5	0.59	0.46	0.68	0.75	0

Let us consider the following scheme for defining the consonance and dissonance between each pair of criteria (see Table III).

Criteria relation	Obtained $\langle \mu_{C,C'}, \nu_{C,C'} \rangle$ values in case of		
	average results	worst results	best results
$C_1 \leftrightarrow C_2$	$\langle 0.91, 0.08 \rangle$	$\langle 0.79, 0.20 \rangle$	$\langle 0.74, 0.19 \rangle$
$C_2 \leftrightarrow C_4$	$\langle 0.78, 0.21 \rangle$	$\langle 0.84, 0.15 \rangle$	$\langle 0.53, 0.44 \rangle$
$C_1 \leftrightarrow C_4$	$\langle 0.74, 0.26 \rangle$	$\langle 0.88, 0.12 \rangle$	$\langle 0.63, 0.33 \rangle$
$C_3 \leftrightarrow C_4$	$\langle 0.55, 0.44 \rangle$	$\langle 0.33, 0.66 \rangle$	$\langle 0.71, 0.26 \rangle$
$C_1 \leftrightarrow C_3$	$\langle 0.41, 0.58 \rangle$	$\langle 0.34, 0.65 \rangle$	$\langle 0.49, 0.44 \rangle$
$C_3 \leftrightarrow C_5$	$\langle 0.38, 0.60 \rangle$	$\langle 0.64, 0.35 \rangle$	$\langle 0.30, 0.68 \rangle$
$C_2 \leftrightarrow C_3$	$\langle 0.36, 0.62 \rangle$	$\langle 0.18, 0.80 \rangle$	$\langle 0.35, 0.59 \rangle$
$C_2 \leftrightarrow C_5$	$\langle 0.27, 0.71 \rangle$	$\langle 0.22, 0.77 \rangle$	$\langle 0.51, 0.46 \rangle$
$C_1 \leftrightarrow C_5$	$\langle 0.26, 0.74 \rangle$	$\langle 0.14, 0.86 \rangle$	$\langle 0.36, 0.59 \rangle$
$C_4 \leftrightarrow C_5$	$\langle 0.11, 0.89 \rangle$	$\langle 0.07, 0.93 \rangle$	$\langle 0.25, 0.75 \rangle$

In the case of the average values of the examined criteria, in accordance with the scale presented in Table III, we found the following pair dependencies:

- There is no observed strong positive consonance or strong negative consonance between any of the ten criteria pairs. Since the observed values depend on the number of objects if we can expand their number, it is possible to

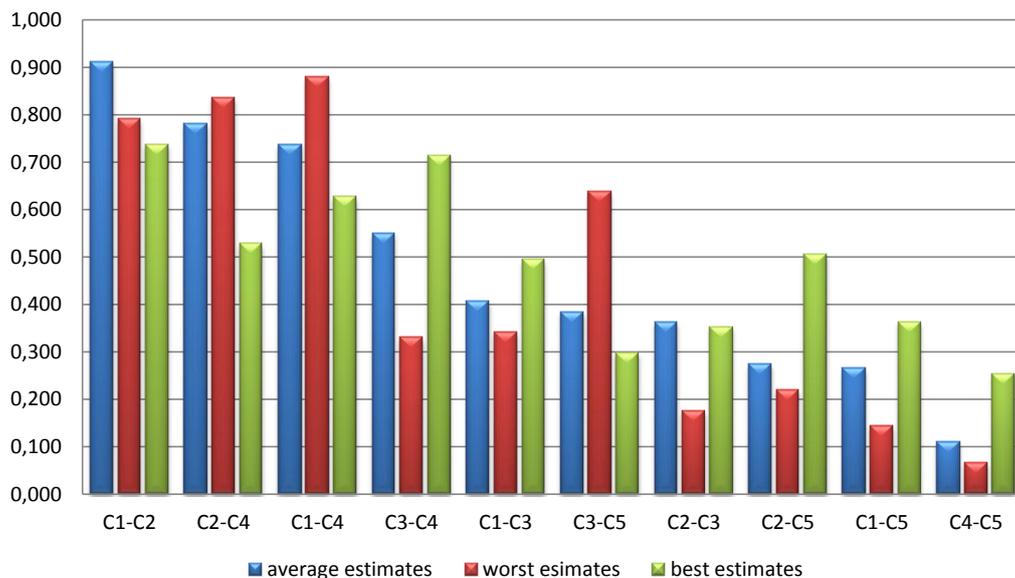


Fig. 1. Degrees of “agreement” (μ_{C,C'} values) for all cases

TABLE III
CONSONANCE AND DISSONANCE SCALE

Interval of μ _{C,C'} , %	Meaning
[0-5]	strong negative consonance
(5-15]	negative consonance
(15-25]	weak negative consonance
(25-33]	weak dissonance
(33-43]	dissonance
(43-57]	strong dissonance
(57-67]	dissonance
(67-75]	weak dissonance
(75-85]	weak positive consonance
(85-95]	positive consonance
(95-100]	strong positive consonance

obtain values in these intervals.

- For the pair C₄ ↔ C₅ (i.e., T ↔ J) a negative consonance is identified. Such dependence is logical – for a large number of algorithm iterations (i.e., greater execution time T) it is more likely to find a more accurate solution, i.e. smaller value of J.
- The pairs C₂ ↔ C₅ (i.e., k_S ↔ T) show identical results – these criteria are in weak dissonance. The third model parameter Y_{S/X} and T are in dissonance. The conclusion is that the total execution time is not dependent solely on one of the model parameters. Logically the triple of these parameters should be in consonance with T.

- For the pairs C₁ ↔ C₃ (i.e., μ_{max} ↔ Y_{S/X}) and C₂ ↔ C₃ (i.e., k_S ↔ Y_{S/X}) a dissonance is observed. Considering the physical meaning of the model parameters [1] it is clear that there is no dependence between these criteria. A strong correlation is expected between criteria C₁ ↔ C₂ (i.e., μ_{max} ↔ k_S) [1]. The results confirmed these expectation – these criteria are in a positive consonance.
- The observed low value of μ_{C₃,C₄}, i.e., strong dissonance between Y_{S/X} ↔ J show the low sensitivity of this model parameter. According to [18] the parameter Y_{S/X} has lower sensitivity compared to parameter μ_{max}.
- Due to the established strong correlation between criteria C₁ ↔ C₂ (i.e., μ_{max} ↔ k_S) we observe that C₁ ↔ C₄ (i.e., μ_{max} ↔ J) and C₂ ↔ C₄ (i.e., k_S ↔ J) are in, respectively weak dissonance and weak positive consonance. Similarly to the relations with T the conclusion is that the accuracy of the criterion is not dependent solely on one of the model parameters. Logically the triple of these parameters should be in consonance (or strong consonance) with the criterion value. Moreover, taking into account the parameters sensitivity it is clear that the more sensitive parameter will be more linked to the value of J.

Due to stochastic nature of considered here GA we observed some different criteria dependences in the rest two cases – case of worst and case of best results:

- In the case of the worst results we found weaker relation between C₁ ↔ C₂, C₃ ↔ C₄, C₂ ↔ C₃, C₁ ↔ C₅, C₂ ↔ C₅ and C₄ ↔ C₅. For the pairs C₁ ↔ C₄, C₂ ↔ C₄ and C₃ ↔ C₅ we observed higher value of μ_{C,C'}. Compared to the case of average results there are no large, strongly manifested discrepancies. In case

of discrepancy, the considered criteria pair appears in an adjacent scale according to Table III. For example, pair $C_1 \leftrightarrow C_2$ in case of average results are in positive consonance, while in case of worst results – in weak positive consonance.

- In the case of the best results we identify the same results – in case of discrepancy the considered criteria pair appears in an adjacent scale. However, in this case we observed some larger discrepancies. Taking into account the nature of the GA we consider that the results in case of average criteria values have the highest significance.

V. CONCLUSION

In this paper based on the apparatus of the Index Matrices and the Intuitionistic Fuzzy Sets, InterCriteria Analysis of a model parameters identification using Genetic Algorithm is performed. A non-linear model of an *E. coli* fed-batch cultivation process is considered. Series of model identification procedures using Genetic Algorithms are done. The InterCriteria Analysis is applied to explore the existing relations and dependencies of defined model parameters and Genetic Algorithms outcomes – execution time and objective function value. Three case studies are examined – considering average, worst and best results for the obtained model parameters, execution time and objective function value. Applying the InterCriteria Analysis we establish relations and dependencies between the defined criteria. Based on the used scale for defining the consonance and dissonance between each pair of criteria, we discuss which criteria are in consonance and dissonance, as well as the degree of their dependence.

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