

Interpolation and Exploration of Response Surfaces using Evolutionary NURBS, LaGrange Constraint and Cylindrical Operators

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ABSTRACT

In this article, a computational model for the interpolation and exploration of Complex Response Surfaces is described and analyzed. This computational model consists of two stages: an initial stage in which a group of measured points is interpolated by means of the coalition of characteristic concepts of vector geometry, numeric methods and evolutionary computation to construct a response surface; and a second stage, where a series of good trajectories by means of the exploration of the interpolated surface are determined. In this stage, an evolutionary algorithm, processing a mutation operator that incorporates the fundamental concepts of the cylindrical coordinates, is used to identify a trajectory containing the best combinations among the variables of the particular process this surface represents.

Categories and Subject Descriptors

I.3.5. [Computer Graphics]: Computational Geometry an Object Modeling – *Curve, surface, solid and object representations; Splines*. I.2.1 [Artificial Intelligence]: Applications and Expert Systems. J.2 [Computer Applications]: Physical Sciences and Engineering – *Engineering*.

General Terms

Algorithms, Design.

Keywords

Optimal Surface Interpolation, Evolutionary Algorithms, NURBS, LaGrange Constraints.

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1. INTRODUCTION

The emulation of the behavior of many natural phenomena using computational tools has been very little developed, mainly because many of the tools based on computational intelligence were conceived, in its time, for very precise and defined technical problems. Leaving aside incomplete or blurred information treatment as it is presented in the many phenomena of growth of plants and living beings.

The study of these phenomena of growth has been modest during decades and the approaching made through time using formal methods of experiments design, have had as main objective the identification of the phenomenon's variables through lineal models. Natural phenomena are not-linear; a clear example is the edible and medicinal funguses growing, which are produced under specific conditions depending of the weather of each country, available sow, and local practices.

In this paper, the construction of the response surface for the growth of the mushroom *Pleurotus ostreatus* in one of its first stages of growth is presented. For the construction of the response surface, the *pH* (Acidity of the Sow) and time (*t*) were taken as independent variables, while the answer variable will be the geometrical growth of the mushroom. Other traditional models, with higher order, have shown very low levels of confidence, 45% to 50% of prediction, because the noise and the complex behavior observed in the data points used for the analysis. Additionally, with experiments design methods, model building and the exploration of a multimodal surface requires a lot of time [8]. To increase the levels of dependability in the found patterns is necessary to obtain response surfaces with polynomial functions that represent in a more precise way the relationship among the variables that compose the real pattern, with the limitation that the polynomial degree grows according with the quantity of available points for building the surface.

To eliminate many of the problems found with traditional approaches of experiments design, a new evolutionary method has been developed. Our new method for obtaining response surfaces uses concepts of evolutionary computation fused with

concepts of interpolation surfaces by NURBS (Non Uniform Rational Basis Splines) and LaGrange Interpolation. Starting from the analytic obtaining of tracts of the surface, a uniform unfolding of the same one is made in a series of triangular planes, which indicates sectors where lineal relationships among the variables exist. Then, beginning from this unfolding, a pattern model is developed using characteristics of the evolutionary computation and concepts of cylindrical coordinates. This novel model allows obtaining good trajectories over the surface with the best combination of values among the variables composing the specific response surface.

For the understanding of the pattern development, this article begins with the basic concepts of the interpolation with NURBS and their coalition with elements of the evolutionary computation. Then, cylindrical coordinates and the evolutionary computation coalition for the development of a mutation operator of cylindrical type to navigate on the surface is presented. Finally, for the validation of the response surface evolutionary model, this is applied to the growth of the mushroom type *Pleurotus ostreatus*, under different *pH* conditions, in one of its first stages of growth.

2. INTERPOLATION OF CURVES AND SURFACES WITH NURBS (TRADITIONAL FORM)

A brief summary of the interpolation of curves and surfaces using NURBS is presented. A detailed description of this interpolation form can be in [2], [4].

2.1 Surfaces and Curves NURBS (Non Uniform Rational Basis Splines)

A NURBS curve is defined in the following way:

$$C(u) = \frac{\sum_{i=0}^m w_i P_i N_{i,p}(u)}{\sum_{i=0}^m w_i N_{i,p}(u)} \quad (1)$$

Where $\{w_i\}$ are denominated weights, $\{P_i\}$ are the points of control of the interpolation, while $\{N_{i,p}(u)\}$ are basic functions normalized, B-Splines of the grade p . The weights w_i determine the influence of the vector i -th of control P , on the curve. The i -th basic functions $N_{i,p}(u)$ are defined on a vector of knots $U = \{u_0, u_1, \dots, u_{m+p+1}\}$. They are recursively defined in the following way:

$$N_{i,p}(u) = \frac{u - u_i}{u_{i+p} - u_i} N_{i,p-1}(u) + \frac{u_{i+p+1} - u}{u_{i+p+1} - u_{i+1}} N_{i+1,p-1}(u) \quad (2)$$

where:

$$N_{i,o}(u) = \begin{cases} 1 & \text{if } u_i \leq u \leq u_{i+1} \\ 0 & \text{otro caso} \end{cases} \quad (3)$$

The vector of knots is a group of numbers that indicates the beginning and the end of the rational functions. In many cases the rational functions may be of uniform type, for what the vectors of knots can be classified as periodic. If the group of points to interpolate is not equally spaced, the vector of knots is considered non periodic. In the general case, this vector is non-periodic and has the following form:

$$U = \{\alpha, \dots, \alpha, u_{p+1}, \dots, u_m, \beta, \dots, \beta\} \quad (4)$$

where α and β appear $(p+1)$ times at the beginning and at the end. This special arrangement guarantees that the function begins and concludes respectively in the first and last control point. For this particular case the parameters will be defined in the range $u \in [0,1]$ and the weights are ideal when they come closer to the unit.

A NURBS surface is define as the tensile product, in this way:

$$S(u, v) = \frac{\sum_{i=0}^m \sum_{j=0}^n w_{i,j} P_{i,j} N_{i,p}(u) N_{j,q}(v)}{\sum_{i=0}^m \sum_{j=0}^n w_{i,j} N_{i,p}(u) N_{j,q}(v)} \quad (5)$$

where $\{w_{i,j}\}$ are weights, $\{P_{i,j}\}$ are the control points or the points to interpolate and $\{N_{i,p}(u)\}$, $\{N_{j,q}(v)\}$ are the normalized basic functions, B-Splines, defined on the non periodic knot vectors $U = \{0, 0, \dots, 0, u_{p+1}, \dots, u_m, 1, 1, \dots, 1\}$, and $V = \{0, 0, \dots, 0, v_{q+1}, \dots, v_n, 1, 1, \dots, 1\}$ respectively. Here P and Q are the degrees of the interpolation rational functions in the addresses u and v .

2.2 Interpolation of Curves and Surfaces through NURBS.

To determine an interpolation NURBS curve $\{Q_k\}$ for $(m+1)$ given points, these suffixes have $(m+1)$ independent conditions. Assigning a value for \bar{u}_k , to each one of the points to interpolate, and selecting two knots vector, U and W . The interpolation problem is:

$$Q_k = C\left(\bar{u}_k\right) = \sum_{i=0}^m P_i R_{i,p}(\bar{u}_k) \quad \text{para } k = 0, \dots, m \quad (6)$$

Or in matrix form:

$$\begin{bmatrix} R_{0,p}(\bar{u}_0) & \dots & R_{m,p}(\bar{u}_0) \\ R_{0,p}(\bar{u}_1) & \dots & R_{m,p}(\bar{u}_1) \\ \dots & \dots & \dots \\ R_{0,p}(\bar{u}_m) & \dots & R_{m,p}(\bar{u}_m) \end{bmatrix} \begin{bmatrix} P_0 \\ P_1 \\ \dots \\ P_m \end{bmatrix} = \begin{bmatrix} Q_0 \\ Q_1 \\ \dots \\ Q_m \end{bmatrix} \quad (7)$$

Where the rational functions $\{R_{i,p}(u)\}$ are defined as:

$$R_{i,p}(u) = \frac{w_i N_{i,p}(u)}{\sum_{i=0}^m w_i N_{i,p}(u)} \quad (8)$$

In surface treatment, the knots vector for the addresses u and v will be determined by an arrangement $(m+1) \times (n+1)$ of points $\{Q_{k,l}\}$ to interpolate with $k = 0, \dots, m$ and $l = 0, \dots, n$. The Interpolation of a surface from an arrangement of given points can be expressed by means of the equation (9).

$$Q_{k,l} = \sum_{i=0}^m \sum_{j=0}^n P_{i,j} R_{i,p}(\bar{u}_k) R_{j,q}(\bar{v}_l) = \sum_{j=0}^n \left[\sum_{i=0}^m P_{i,j} R_{i,p}(\bar{u}_k) \right] R_{j,q}(\bar{v}_l) \quad (9)$$

$$= \sum_{j=0}^n C_j(\bar{u}_k) R_{j,q}(\bar{v}_l)$$

3. EVOLUTIONARY INTERPOLATION SURFACES.

The conventional methods of parameterization, in the most cases, are inadequate to generate NURBS free surfaces that follow a behavior of the convex hull, formed by the interpolation points. For this reason, a new approach for the interpolation it is established as: The values of the parameters for each interpolation point are taken as the maximum value of each randomly-generated rational function.

The rationale for this parameterization heuristic is explained as follows. If the evaluation of the parameters is grouped against the rational functions, a matrix is obtained with dominant elements in the main diagonal. For this reason, when taking the parameters of the vector of knots like the point where the maximum of these rational functions is, the inverse matrix of R with dominant elements in the main diagonal is obtained. This assures that fallacious bends are not obtained when generating the best interpolation curve.

3.1 Generation of the Rational Functions.

Rational functions $R(u)$, conformation that will be directly bound to the individual who evolves inside the evolutionary algorithm of interpolation.

The basic rational function is conformed by 6 points, where each point will be conformed by two coordinates (u_i, y_i) , where the u_i values will be given by the traditional formula of partition of axes, while the values of y_i will be located inside the evolutionary individual. For the previous particular case of 6 points, the individual will be conformed as it is shown in the Figure 2 according to Figure 1.

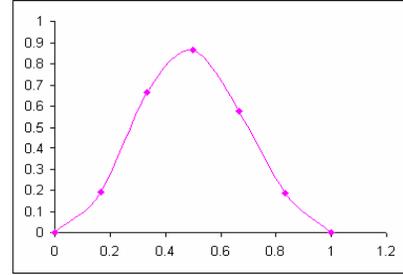


Figure 1. Conformation of the rational base functions $R(u)$.

In figure 1, each one of the points over the rational function is located on the knots vector. These points have a height given by the vector in figure 2:

y_0	y_1	y_2	y_3	y_4	y_5	y_6
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Figure 2. Height for the structure conformation of the rational functions $R(u)$.

Each rational function has an equation as:

$$R(u) = y_0 L_0(u) + y_1 L_1(u) + \dots + y_n L_n(u) \quad (10)$$

where:

$L_i(x)$: LaGrange polynomial, depending of the m values that conforms the knots vector, where the rational functions are linked.

$$L_i(u) = \prod_{j=0, j \neq i}^m \frac{u - u_j}{u_i - u_j} \quad (11)$$

The line that unites the points that conform the rational functions is given by a polynomial of order n (for the rational function of the Figure 1, $n = 6$). For the case of polynomial union of smaller degree, polynomial functions can settle down for segments. It is remarkable that the knots will be located in the extreme of the rational function, while the point to be interpolated will be found exactly above the central point; the other points are result of a uniform partition of the rational functions derived from the conformation of the rational functions. For an interpolation of a group of nine points the rational functions may take the form in Figure 3:

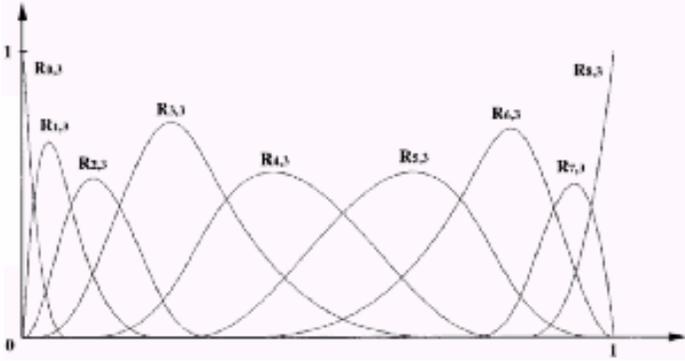


Figure 3. Rational Functions of order 3, for the interpolation of 9 control knots1.

The total numbers of points for the conformation of the rational functions of a whole of n interpolation points is calculated with equation (12):

$$(n + 1) * 7 - 12 \quad (12)$$

3.2 Evolutionary Algorithm of Interpolation.

Beginning with the surface interpolation, it is necessary to keep in mind the following points [7], [8]:

An appropriate partition for the vector of knots that determine the beginning and final of each one of the rational functions to be generated.

An initial population of individuals where each one of the genes will represent each one of the points that conforms the rational functions mentioned in the point 3.1[3].

After the initial population definition, we apply the following evolutionary operators [5]:

1. The *Selection Operator of Roulette* chooses for the following generation the population's better individual.
2. The *Operator of Recombination, elitism with replacement*, where the best individual participates in all crossovers.
3. The *Operator of Mutation* uses an evolution strategy where a gene is chosen in a random way. To each gene selected for the mutation a random number is added or subtracted while the fitness function of each individual improves.

3.3 Fitness Function of the Interpolation Algorithm.

For the evaluation of the individuals the following procedure is applied [7], [8]:

1. Build the rational functions for each individual and determine the equation of each one of them to obtain the matrix R .
2. Find the Euclidean distance among the real points and the generated points by the interpolation matrix R (the knot vector and their secondary partitions will be static during the evolution process). In accordance with the above-mentioned the fitness function for this case will be given by the equation (13).

$$D = \sqrt{\sum_{j=0}^m (P_j - Q_j)^2} \quad (13)$$

Where:

D : indicates the Euclidean distance among the data point (P_j) and the generated points (Q_j) by the matrix R .

Avoiding obtaining missed interpolation functions or overflow of the rational functions between point and point, it is necessary to include inside the fitness function a part that limits the growth of the rational functions. This constrain will be given in this way:

1. The proposed main and secondary partitions are evaluated for the construction of the rational functions against the interpolation matrix.
2. A series of LaGrange functions are selected to interpolate the main points of the surface in the sense of each one of the variables.
3. The secondary points are evaluated according to the LaGrange interpolation polynomial. The difference among the values given by the matrix of interpolation and the values given by the evaluation of the polynomial of LaGrange is calculated to obtain the value L .

In the general case, with n partitions in the unfolding of the response surface, the fitness function is determined by a LaGrange Constraint of n order, as follows:

$$p(x) = f(x_0)L_0(x) + f(x_1)L_1(x) + \dots + f(x_n)L_n(x) \quad (14)$$

where:

$L_i(x)$: LaGrange polynomial, depending of n surface partitions.

$$L_i(x) = \prod_{j=0, j \neq i}^n \frac{x - x_j}{x_i - x_j} \quad (15)$$

This polynomial has a different order respect to the total number of points, since the LaGrange constraint takes in account only the surrounding values to the point, needed to error calculation. Obtaining information about the height of the neighbor points of the evaluated point increases the power interpolation.

By this way the fitness function for each one of the population's individuals will be given by the equation (16) [8]:

$$FA : \frac{1}{\alpha D + \beta L} \quad (16)$$

Where:

FA : Fitness Function Value.

¹ Jung, H.B., Kim K. *A New Parameterization Method for NURBS Surface Interpolation*. Advanced Manufacturing Technology. Springer-Verlag, London, 2.001.

L : LaGrange Error.

α, β : Weight Factors (factors allowing the values L, D , have the same order of magnitude).

x_i, x_j : Interpolation Original Points.

4. EVOLUTIONARY NAVIGATION ON THE INTERPOLATED RESPONSE SURFACE.

So far, the first stage of the evolutionary method of interpolation and exploration of a response surface originated in a data point set has been presented. This process consists in the modification of the traditional NURBS method with an evolutionary algorithm that locates the maximum value of each randomly generated rational function in each interpolation point. After this, the evolutionary algorithm is enriched with LaGrange functions, reflecting the variables action, to correct the secondary points in order to follow an adequate behavior in the convex hull.

The second stage is the navigation on the interpolated surface to identify good trajectories with the best combination of the variable's amounts. Due to the conception of the selection and recombination operators inside the algorithm, the identification and crossing of information among the population's individuals is achieved, while the exploration of the surface is carried out with the mutation operator by means of the use of the geometric concept of cylindrical coordinates [1]. To determine those trajectories, the same structure of the interpolation evolutionary algorithm will be used according with the operators of selection by roulette and the operator of recombination.

For the first stage, a non evolutionary behavior, an experiments design, and an evolutionary process were generated, in which there was not any approach for a behavior, neither for the allowed ranges for the modification of the values of the independent variables. This means that in many cases the found behavior will not identify the best combination of values neither the maximum points inside the response surface [1]. The second stage is completely evolutionary and is responsible to get the best combination in values of the variables of the process the response surface represents. The interpolation and exploration evolutionary algorithm was applied to emulate the growth process of the mushroom *Pleurotus ostreatus*.

4.1 Cylindrical Evolutionary Mutation Operator.

The mutation operator is in charge of identifying the areas of the interpolated response surface where a given behavior of the phenomenon is detected.

In the case of the growth process of the mushroom *Pleurotus ostreatus* a gradual and always increasing growth, with the smallest pH variation, was observed. Starting from the non evolutionary process, that general behavior of the trajectory for the particular case of the growth of the mushroom *Pleurotus ostreatus* was identified and following from here the value of the independent variables were taken. This is time in days (t) and the pH value (acidity of the sow) for every day. In accordance with this, the proposed emulation evolutionary algorithm fixes

the string of genes that contains the values of the days, and goes modifying the values of the other variable (pH), so that between day and day will exist a controlled growth with moderate variation of the independent parameters [9].

For this case, a set of mutation positions inside the whole of the individuals' genes was generated and the concept of coordinated cylindrical is used to identify the best vicinities for the gene selected for the mutation, these better vicinities are determined by a bigger value to the value considered for the point of mutation.

According to this mutation strategy the gene previous to the gene selected for the mutation will be chosen, gene that we will call central point and that it will be represented by the coordinates:

X_c : Central day for the mutation.

Y_c : Central pH for the mutation.

With these coordinates a value, called F_c , could be calculated. The positions that were selected for the mutation will be denoted in the following way:

X_a : Day to change during the mutation.

Y_a : pH to change during the mutation.

For these coordinates a specific value is also calculated, denoted as F .

For the mutation, the central point is taken and a sector of arch of approximately 90° with a variation of 15° is considered around the central point as it is shown in the equation (17).

$$\begin{aligned} \varphi &= 0.2617993 * i, \quad x_2 = x_c + r * \cos(\varphi), \\ y_2 &= y_c + r * \sin(\varphi) \end{aligned} \quad (17)$$

Where:

x_2 : represents the new point for the coordinate days.

y_2 : represents the new point for the coordinate pH.

φ : Variation angle or variation allowed for the independent variables.

$r = \frac{1}{NP}$: Radio of the circular sector on which is carried out the advancement.

NP : Number of steps for the emulation path.

i : random value of the angle variation of the circular sector, this value will be delimited in the interval [-3,3], where 0.261793 are approximately 15° in radians.

For this point a value of the growing behavior will be evaluated, and it will be denoted F_2 .

In accordance with this, if the value $F2$ overcomes as minimum the value of $(1/NP)*CF$, the values of the coordinate (Xa, Ya) are modified respectively in the algorithm by the values of $(X2, Y2)$

This way, and in accordance with the aptitude values, makes sure that the behavior of the phenomenon will be made in gradual and always growing way upon some given conditions and in correspondence with the variations that it can suffer under its pH conditions [1].

5. RESULTS VALIDATION.

For the validation of the model it was taken into account the growth of the mushroom *Pleurotus ostreatus* in one of its first stages of growth. For the construction of the response surface, the pH (Acidity of the Sow) and time (t) were taken as independent variables, while the answer variable will be the growth of the mushroom, C , cultivated in plates of Petri of 10 cm of diameter.

To achieve the validation of the model are necessary two fundamental stages of the pattern, they are:

1. Evolutionary interpolation of the surface.
2. Evolutionary emulation for the growth of the mushroom.

For the evolutionary interpolation of the surface the most successful growth achieved in laboratory by the mushroom was chosen, in this case the sow PDA (Potatoes, Dextrose and Agar). In Figure 5 two overlapped lines are shown, one indicates a border of the surface of data points, while the other line indicates the interpolation line for the same data [9].

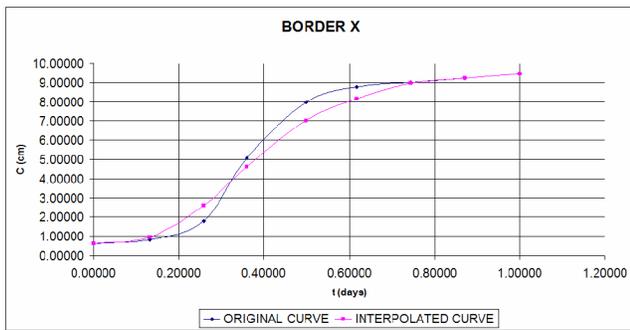


Figure 4. Lines including the termination criteria for the Evolutionary Interpolation.

To determine the magnitude of the interpolation it is necessary to show a superior view of the surface to observe the contours of the growth that indicate the form in which the interpolation was made.

The numeric results obtained for the considered sow were the following ones:

1. Iterations Number: 150.
2. Individual fitness: 51.23.
3. Interpolation Mesh Error: 1.95 cm. (81 points).
4. Confidence Percentage: 99.76%.

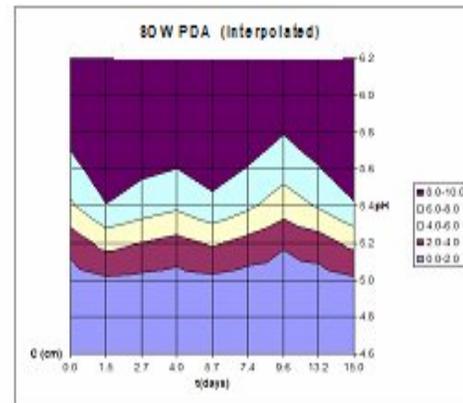
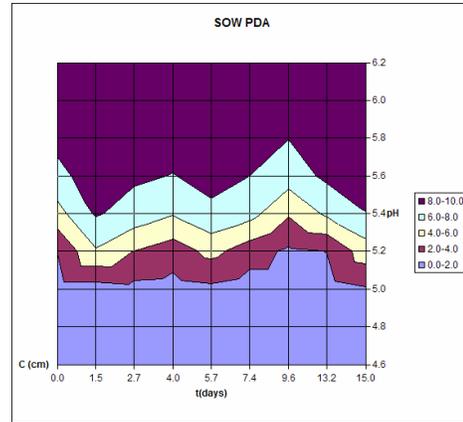


Figure 5. Top view of the data points surface and the interpolated Surface.

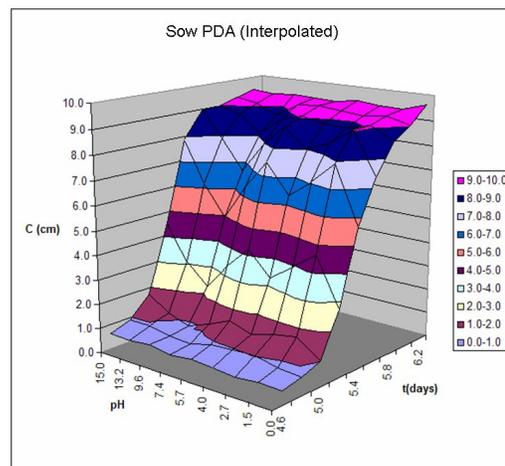


Figure 6. Interpolated Surface.

To achieve an emulation that reflects in a real way the growth of the mushroom, the response surface had to be triangled in a uniform way, so that the lineal confidence of the triangular surface with regard to the analytical response surface was [9]:

1. For 81 points: 82.16%
2. For 324 points: 87.84%
3. For 6556 points: 96.61%.

The validation of the model of evolutionary emulation (or exploration) was achieved identifying the *pH* values common to each one of the growths found by the evolutionary interpolation method and then carrying out experimentation in the laboratory again with those *pH* values that presented a successful growth. From the analysis of the data a gap for each sow in each one of the days of the observed mushroom growth was registered, then an average gap and a value of variance point to point for the whole stage of the mushroom growth considered in this model was calculated [9].

Table 1. Evolutionary Growth vs. Growth of validation Comparison, sow PDA.

PDA						
Day	pH	C (cm)(EE)	C (cm)(V)	DIF.	MEDIAN	VARIANCE
0.00	4.93	0.54	0.65	0.12	0.09960853	0.34845489
0.65	5.71	0.65	0.73	0.08		
1.72	5.50	0.71	0.74	0.03	TOTAL ERROR	
2.79	5.70	0.94	0.82	-0.11	-3.54	
3.95	5.34	1.24	1.17	-0.07		
5.58	5.81	2.90	2.84	-0.06	% ERROR	
6.84	5.16	5.72	5.17	-0.55	0.99608528	
7.91	5.87	6.53	6.36	-0.17		
9.86	5.12	6.92	8.66	1.74		
11.84	4.90	6.77	7.12	0.35		
13.21	5.30	9.43	9.18	-0.26		

For this type of sow, the growth presents a total error of 3.54 cm in all the points considered for the growth of the mushroom. The average of the error with regard to a total diameter of 10 cm was of 0.099cm, a Petri plate of 10 cm was the patron measure for the mushroom growth. The standard deviation of the data was found around 0.34845 cm, with regard to the average.

The evolutionary model, here presented, was tested against the model proposed in [6]. In this model, the combination of effects from temperature and propionic acid for the *Aspergillus parasiticus* are evaluated. Figure 7 shows the behaviours obtained in [6] and the evolutionary model for a temperature $T=36^{\circ}\text{C}$.

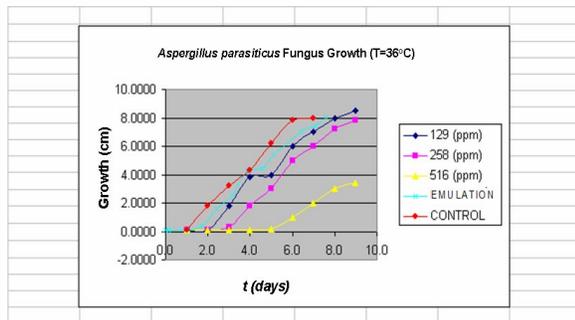


Figure 7. *Aspergillus parasiticus* Fungus Growth ($T=36^{\circ}\text{C}$)

The three lower curves represent experimental processes. The upper curve is the optimal growing interpolated in [6], while the

fourth curve was obtained by the evolutionary model, according to table 2.

Table 2. Evolutionary Growth vs. Growth of validation Comparison, sow PDA.

t (days)	ppm	C(cm)	t (days)	C(cm)	Median
0.0	255.33	0.10	0.0	0.1	0.47
0.1	268.56	0.10	0.1	0.1	
1.1	308.34	0.10	1.1	0.1	Variance
1.7	259.06	0.34	1.7	1.6	0.20252109
2.4	413.77	1.60	2.4	2.1	
3.1	436.63	2.49	3.1	3.2	
3.9	151.06	4.24	3.9	4.1	
4.6	266.06	4.45	4.6	5	
5.1	257.69	5.41	5.1	6.2	
6.4	264.83	7.04	6.4	8	
7.1	274.42	7.39	7.1	8.2	
7.6	135.56	8.06	7.6	8.3	

6. CONCLUSIONS.

1. The interpolation of a group of data point obtained in laboratory using evolutionary NURBS (Non Uniform Rational Basis Splines), presents a very good approximation point to point.
2. Although this approximation presented some problems of overflow of the data, mainly produced in the NURBS method because the limitless growth of some rational functions among each one of the data point [9], the enrichment of the evolutionary algorithm with LaGrange functions resulted in an adequate solution.
3. The interpolation of the validation case (mushroom growing) using a non evolutionary method presented many deficiencies in regard with the real behavior, because many of the emulated values did not have a relative continuity among the values of the independent parameters (*t*, *pH*). On the other hand, the incorporation of geometrical features in the fitness function allows that the evolutionary emulation presents moderate values of growth with regard to moderated change in the values of the independent parameters; this made the gain for the emulated behavior to be much more gradual.
4. With the evolutionary model of interpolation is easier to find optimal points than the traditional methods for the exploration of response surface, which produces different paths for different weather conditions, and with gradual changes in the controlled variables.

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