

Response Surface Methodology and its application in evaluating scientific activity.

EVARISTO JIMÉNEZ-CONTRERAS,^a DANIEL TORRES-SALINAS,^{a,b} RAFAEL BAILÓN MORENO,^a ROSARIO RUIZ BAÑOS,^a EMILIO DELGADO LÓPEZ-CÓZAR^a.

^a *Evaluación de la Ciencia y la Comunicación Científica, Facultad de Biblioteconomía y Documentación*

Departamento de Biblioteconomía y Documentación, Universidad de Granada, Granada (Spain)

^b *Centro de Investigación Médica Aplicada (CIMA), Universidad de Navarra, Pamplona (Spain)*

The possibilities of the Response Surface Methodology (RSM) has been explored within the ambit of Scientific Activity Analysis. The case of the system “Departments of the Area of Health Sciences of the University of Navarre (Spain)” has been studied in relation to the system “Scientific Community in the Health Sciences”, from the perspective of input/output models (factors/response). It is concluded that the RSM reveals the causal relationships between factors and responses through the construction of polynomial mathematical models. Similarly, quasi-experimental designs are proposed, these permitting scientific activity to be analysed with minimum effort and cost and high accuracy.

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Introduction

The scientific activity focusing on the economic input/output model—especially when dealing with institutions—is classical and almost the foundation of scientific evaluation (MARTIN et al., 1983). This model implies that the system under study has easily defined borders affected by a set of factors or variables called *inputs* and which represent the resources of the system (funding, researchers, equipment, etc.). This system in turn generates or responds to products resulting from their scientific activity, called *outputs*, such as publications or patents.

The relationships which link inputs with outputs are complex and difficult to describe with elemental mathematical models. Therefore, the need arises for tools that are capable of more complex modelling and that achieve maximum refinement of the role of each variable in the system as well as the of synergetic and/or antagonistic interrelationships between the same variables.

The Response Surface Methodology (RSM) emerged in the 1950s (BOX et al., 1951; BOX et al., 1951) within the context of Chemical Engineering in an attempt to construct empirical models able to find useful statistical relationships between all the variables making up an industrial system. This methodology is based on experimental design with the final goal of evaluating optimal functioning of industrial facilities, using minimum experimental effort. Here, the inputs are called factors or variables and the outputs represent the response that generates the system under the causal action of the factors. Afterwards, the use of the RSM was shown in the design of new processes and products. In recent years it is being applied successfully in other scientific fields such as biology, medicine, and economy. MYERS et al. (2004) has exhaustively reviewed the literature in the sense, describing the developments and applications of this methodology. Very recently, RSM has been used even to validate new experimental methods (JURADO et al., 2003).

Objectives

In this paper, we seek to explore the possibilities of the Response Surface Methodology within the scope of the analysis of scientific activity in order to weight the factors which constitute the input/output model, studying not only the classical equation -- human resources plus economic resources equal scientific results seen through this particular method, but also adding others factors which make up the so called scientific production cycle such as the journal impact factor or the international collaboration.

For this, we shall consider the case of the system “Departments of Health Sciences of the University of Navarre”, which for short we will call “University of Navarre” (UNAV), and its interrelationship with the system “Scientific Community in Health Sciences”, or “Scientific Community” for short (Figure 1).

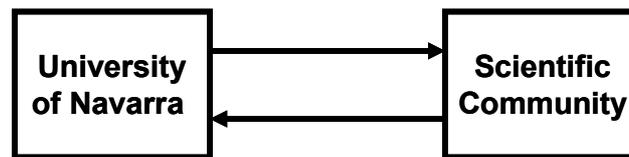


Figure 1. Binomial Departments of Health Sciences of the University of Navarre and the Scientific Community

On the one hand, the University of Navarre will be represented by a system in which the factors (inputs) are the human resources as well as the economic resources while the response (outputs) are the scientific production (Figure 2)



Figure 2. System Departments of Health Sciences of the University of Navarre

On the other hand, the Scientific Community is represented by a system in which the response (outputs) will be the number of citations directed to the UNAV. The prime and essential cause of these citations will be the action of the following factors (inputs): scientific production from this university, the journal impact factor, where this production is published and the degree of international collaboration of the researchers at the UNAV is reflected (Figure 3).



Figure 1. System Scientific Community

Materials and methods

Description of the method of the response surfaces

The designs of the response surface methodology (RSM) are those in which problems are modelled and analysed; in these problems the response of interest is influenced by different variables. The RSM is widely used as an optimisation, development, and improvement technique for processes based on the use of factorial designs—that is, those in which the response variable is measured for all the possible combinations of the levels chosen of the factors. The main effect of a factor is defined as the variation in response caused by a change in the level of the factor considered, when the other ones are kept constant. There is an interaction (dependence) between the variables when the effect of one factor depends on the behaviour of another. The application of the RSM becomes indispensable when, after the significant factors affecting the response have been identified, it is considered necessary to explore the relationship between the factor and dependent variable within the experimental region and not only at the borders. Response surfaces are recommended for these types of factorial designs for their

effectiveness and quick execution. This consists of correlating the k variables put into action through a second-degree polynomial expression of the following form:

$$y_{obs} = b_0 + \sum_{i=1}^k b_i x_i + \sum_{i=1}^{k-1} \sum_{j=i+1}^k b_{i,j} x_i x_j + \sum_{i=1}^k b_{i,i} x_i^2 + e$$

where y_{obs} is the dependent variable, and x_i the factors or variables with which we wish to correlate it. The expression contains a first-degree term that represents a linear relationship considered as the principal, another term in which the variables cross each other to represent the influence of some over others, and finally a second-degree term that refines the previous one and gives maximums and minimums—i.e. optimal values of the dependent variable. The symbols b_0 , b_i , $b_{i,j}$ are constants and e a term of error or residual between the observed and calculated value. The experimental values are adjusted to the above equation by a polynomial regression and the usual statistics can be used to determine the goodness of the fit.

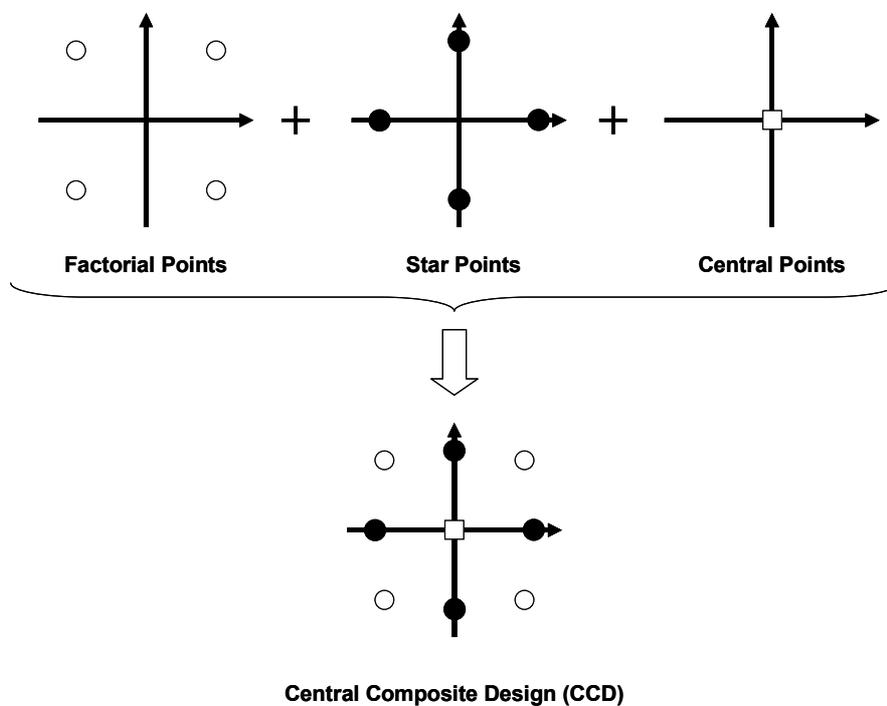


Figure 4. Central Composite Design (CCD) for two factors

The SRM implies, apart from the use of a second-degree polynomial model, a very reduced experimental design called Central Composite Design (CCD) (Figure 4). The CCD is formulated on the basis of the factorial designs adding the star points and the central point, and three types of different structures can be used (Figure 5).

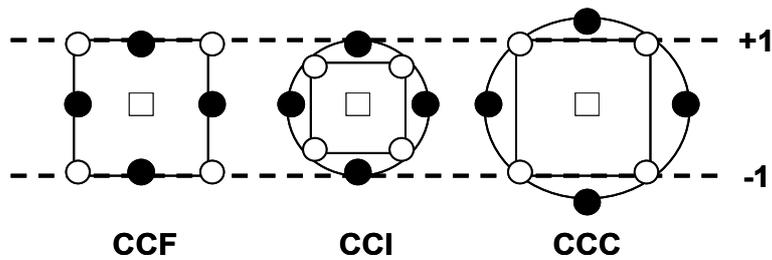


Figure 5. Different structures of CCD: central side (CCF), inscribed (CCI) and circumscribed (CCC)

Regardless of the structure of the composite central design that is used, for each factor or variable, experiments will be performed for 5 different values or levels: $-\alpha$, -1 , 0 , $+1$ y $+\alpha$. Therefore, not all the combinations possible will be made, but rather only those that fulfil a geometric CCD design, i.e. only the points indicated.. In this case of a two-dimensional response surface, they will be shown in Table 1.

Table 1. Selection of values for a response surface

<i>Nº Exp</i>	X_1	X_2
1	-1	-1
2	+1	-1
3	-1	+1
4	+1	+1
5	$+\alpha$	0
6	$-\alpha$	0
7	0	$-\alpha$
8	0	$+\alpha$
9	0	0
10	0	0
11	0	0
12	0	0

In certain applications, the variables cannot take any combination of values, due to certain restrictions. Figure 6 is an example of an experimental window where only in the shaded area, limited by restricting lines, is the design feasible. To facilitate the setting up and fit of the model, a new group of components are defined, these being called pseudo components.

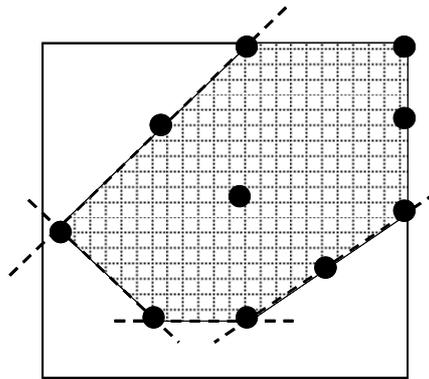


Figure 6. Example of design with restrictions

From the resulting values, for each of the variables, the coefficients of the polynomial equation are determined ($b_0, b_i, b_{i,j}$) and the equation can be simplified according to the influence of the factors in the final response. The resulting equation is used as a model of a given system to determine the response of y as a function of the different values of x_1 and x_2 within the defined area in the CCD, see an example in figure 7.

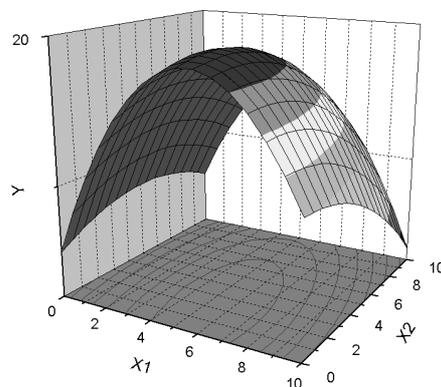


Figure 7. Example of a response surface

To evaluate whether the mathematical model satisfactorily fits the observed data, we first need to analyse the residuals. The model is adequate when the residuals are arrayed without recognizable structure, and thus no obvious pattern would be identifiable.

Through a study of the residuals, many types of misfits to the model and violations of the underlying assumptions can be discovered. Below, to verify the validity of the model, we proceed with the significance test of the regression, the proof of which is made with the F test, comparing the variance of the regression with the residual variance. When the statistical value calculated ($F_{cal} = MQR/MQr$) is greater than the statistical value tabulated ($F_{tab, g, IR, g, Ir}$), we accept the hypothesis that the model chosen is not adequate to describe the experimental data. Another analysis recommended for the evaluation of the goodness of the model is through the R^2 coefficients (explained variability and the Q^2 (predicted variability)). Both coefficients should be near unity and separated by a value close to 0.3.

Table 2. General guide to evaluate the values of the R^2 and Q^2 coefficients

Nature of the data	R^2	Q^2
Chemistry	Acceptable ≥ 0.8	Acceptable ≥ 0.5 Excellent > 0.8
Biology	Acceptable ≥ 0.7	Acceptable ≥ 0.4

Experimental design vs. quasi-experimental design

The experimental designs, as explained above, represent the empirical support of the response surfaces. In the case of a controllable system in a laboratory, the planning and execution of an experimental design implies no more problem than that inherent in the experimentation itself.

On the other hand, if we wish to use the RSM in the evaluation of scientific activity, we must introduce certain novelties into the methodology. In the evaluation of scientific activity, there are no true experiments but rather only observations, and therefore the experimental design, in principle, would make no sense. Although the scientific activity cannot be manipulated in the sense in which variables of physicochemical phenomena are manipulated in a laboratory, they can be selected. That is, we will construct what we will call from here on quasi-experimental designs, which are governed by the same rules as experimental designs, but with specially chosen observations from among the total set of them, in such a way that we find the closest possible values that an experimental design would require. Admitting this, we find that the RSM is feasible. Statistics such as R^2 , Q^2 , etc., thus confirm the validity of the quasi-experimental design proposed.

Material: Area of Health Sciences of the University of Navarre

An evaluation was made of the international scientific production of 50 departments of the University of Navarre (UNAV) related to Biomedicine and Health Sciences in the period 1999-2005. The production data and citations were taken from the Web of Science and those of impact from the Journal Citation Reports corresponding to this period. On the other hand the information on economic and human resources was provided by this university (see Table A in the Appendix). Table 3 presents the variables that have been analysed in this work.

Table 1. Variables analysed in the evaluation of the UNAV

Indicators
N° of researchers
Funding through research projects
N° of works in the databases of Web of Science
N° of citations
% of publications published in the first quartile
N° of members (collaborating institutions)

Overall, the UNAV produced a total of 2,229 works that have received a total of 19,716 citations. Some 41% of their works have been published in journals in the first quartile. Furthermore, there were 822 different collaborating institutions, of which 86% were in the EU and USA. The economic resources identified come from the funding of 534 research projects classified into 5 typologies: Europeans (4%); International (1%); Internal (17%), and Regional (40%). It is assumed that the human resources for the period analysed had an annual mean of 764 full-time researchers, of which 485 were doctors and the rest pre-doctoral and grant students.

For the calculation of the response surfaces, a specific program was used, Modde v. 4, of the company Umetrics of Sweden (www.umetrics.com)

Results and interpretation of the results

System “University of Navarre”

For the calculation of the response surface of the system “University of Navarre” (UNAV), we used a CCF design with restriction, as shown in Figure 8. The cloud of points represents the group of departments in the area of Health Sciences of UNAV. The points highlighted are those departments that have the characteristics closest to the CCF type of design with restrictions.

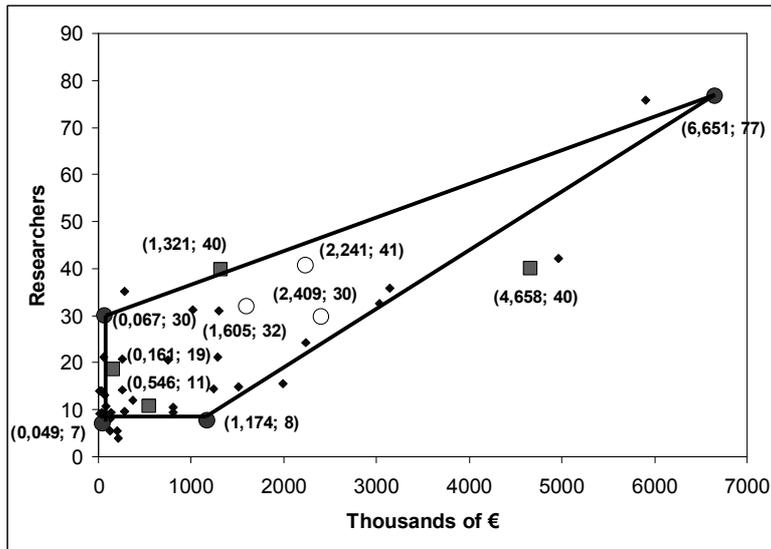


Figure 8. CCF design with restrictions for the UNAV system

The factors used are the number of researchers, S , and the funding, in the form of decimal logarithm, $\log F$ (F is expressed in thousands of €). The response is evaluated as production, P , of scientific articles listed in the Web of Science. The best fit corresponds to a linear response with respect to the number of researchers, while with respect to the logarithm of the funding the response is simultaneously linear and quadratic. There is also a response with respect to the interaction researchers-funding, which signifies that there is a synergetic effect between the two factors.

$$P = 233 - 2.6S - 191 \log F + 44(\log F)^2 + 1.25S \log F \quad R^2 = 0.865 \quad Q^2 = 0.722$$

Eq. 1

The goodness of the response surface represented by Eq. 1 is acceptable. In fact, in agreement with Table 2 and the values of R^2 and Q^2 , the model found is acceptable. On the other hand, the F test of Snedecor confirms also that the fit is satisfactory at the significance level of 5%.

In the same order of things, the set of observed values (production of the departments of UNAV) were compared against the expected ones. The cloud of points is distributed homogeneously on both sides of the regression straightline, which has a slope close to unity (Figure 9).

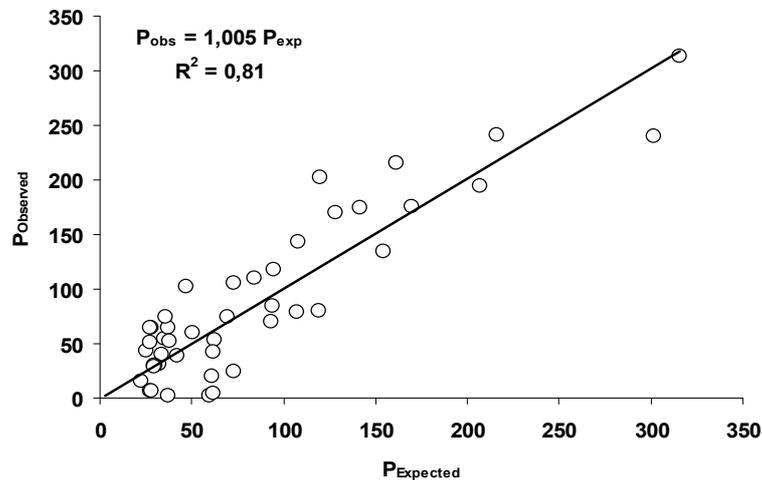


Figure 9. Observed values against the expected ones in the University of Navarre system

However, perhaps the most interesting aspect, from our viewpoint, is the generation of a graphic model that synthesises the weight of the variables chosen and their influence on the results as these variables are changed. There are two basic representations of the model: flat and contour (Figure 10), and three-dimensional or superficial (Figure 11).

From the flat and the three-dimensional representation, it is now easier to explain the behaviour (response) of the scientific system of the UNAV according to whether the factors affecting the production of articles of the departments are affected or not.

Tendency one (Movement 1) shows what happens in the system when, under low funding, the number of researchers increases. Although it may proved unexpected, the result predicts a fall in scientific production. The explanation, however, proves attractive, when the resources are scarce, the increase in staff would prove counterproductive inasmuch as, with decreasing research funds as a consequence of the increase in researchers to attend, the capacity of

producing new works tends to diminish (dark-blue fringe), as insinuated in the lower-right corner. Nevertheless, the capacity of the model in this sphere should not be exaggerated due to the scarcity of the data at this level, to their variability

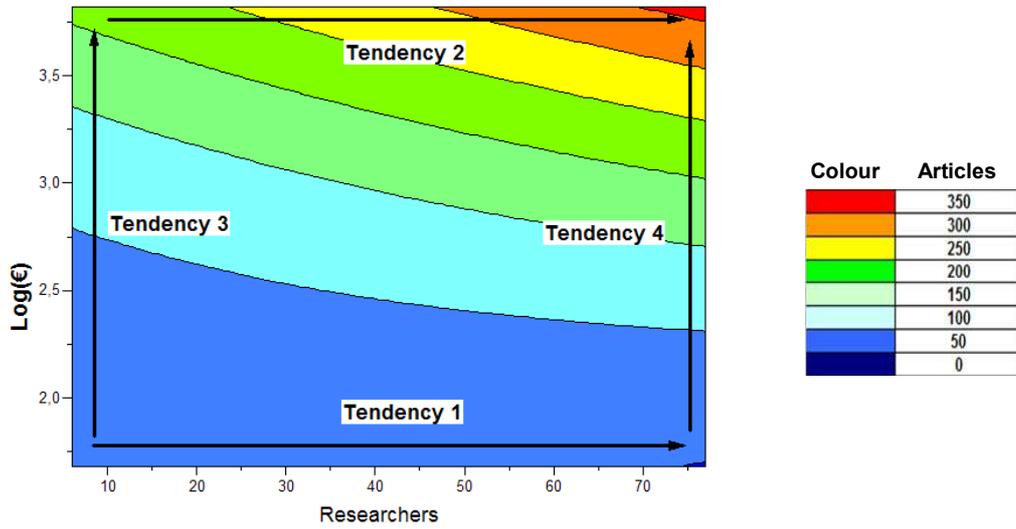


Figure 10. Flat or contour representation for the system University of Navarre

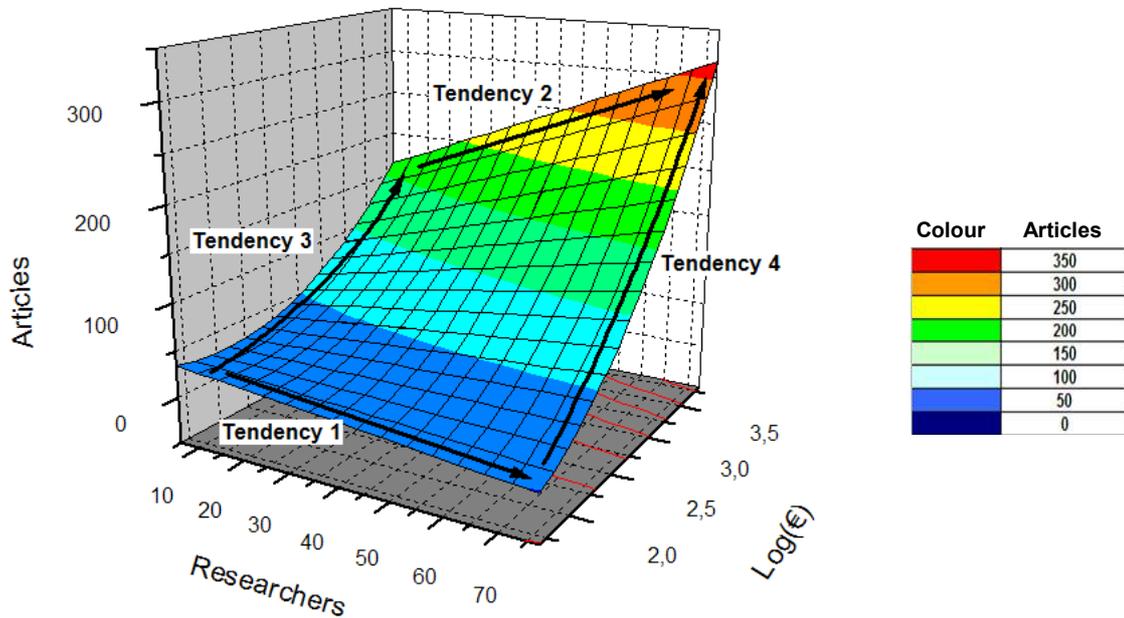


Figure 11. Three-dimensional representation of the surface of the system University of Navarre

Tendency three shows the evolution in the situation of increasing funding with comparatively lower increases in staff. The possible situations covered by the blue and green segments show a progression in the results that even triple those obtained with low funding. Finally, large increases of investment are accompanied by an exponentially greater response, especially in the final part of the graph.

Finally, *tendencies two and four*, which begin with few researchers having abundant financing and many researchers with little funding, the two groups converging in the form of many researchers with much funding. This inevitably marks a similar trajectory that culminates at the maximum limit of the results found in the case of the UNAV. However, the trajectories are not identical; in the first case the path is longer, given that it begins from a more deficient situation. In this sense, the general topography of the sample surface shows that it is far more effective to have fewer human resources with better funding, than the contrary case. In other words, the economic variable is determinant in the human.

System “Scientific Community”

In the second stage, we again apply the same methodology to the system “Scientific Community”, but with the intention of evaluating the impact that the system UNAV has over this community. The response will now be the number of citations, CI, directed to the system UNAV, and the factors used are:

1. Production of scientific articles of the system UNAV: P
2. Position of the journals in which the articles are published, within the impact ranking, or more concretely their presence or absence in the first quartile of the respective categories: J.

3. Collaboration of the authors with international teams, measured by the presence or absence of co-authors from other countries in the teams (partners) I: results are shown in table A (Appendix).

In this case, the goodness of the model, and consequently its predictive capacity prove even greater than in the case of the system UNAV. For example, Figure 12 reflects the perfect alignment between the observed citation values and the expected ones, practically there isn't a residue, that is unexplained variation. That is, the model represented by Eq. 2 is capable of predicting with precision the number of citations that will be received by a certain department of UNAV.

$$CI = 0.014J + 1.6 \times 10^{-5}I + 4,3 \times 10^{-7}P + 0.51P^2 + 0.006JI + 0.41IP \quad R^2 = 0.99 \quad Q^2 = 0.98$$

Eq. 2

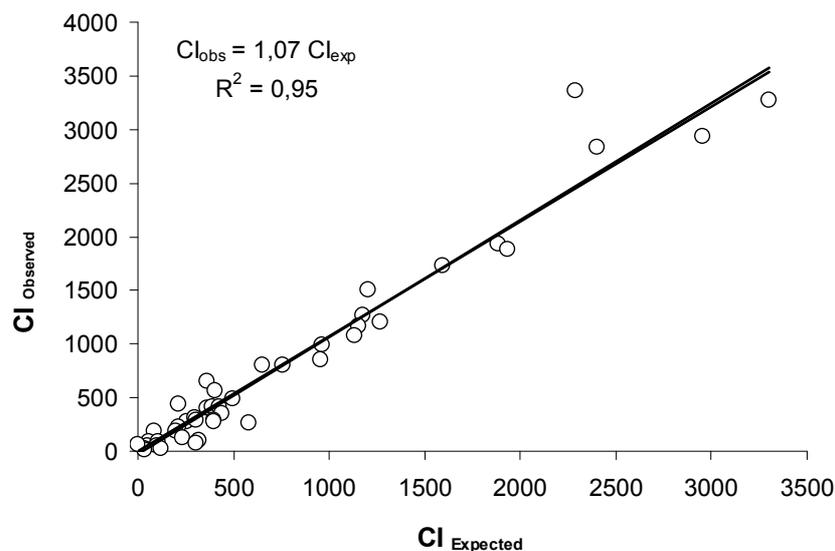


Figure 12. Observed vs. expected values in the system “Scientific Community”

To verify more clearly the respective weights of each variable considered, we considered three possible solutions: departments that do not publish in journals of the first quartile, departments that publish around a third of their works in the first quartile (37%), and, finally, departments that publish about 75% of their articles in the first quartile.

The resulting figures of these three scenarios indicate, respectively (figures 13 and 14):

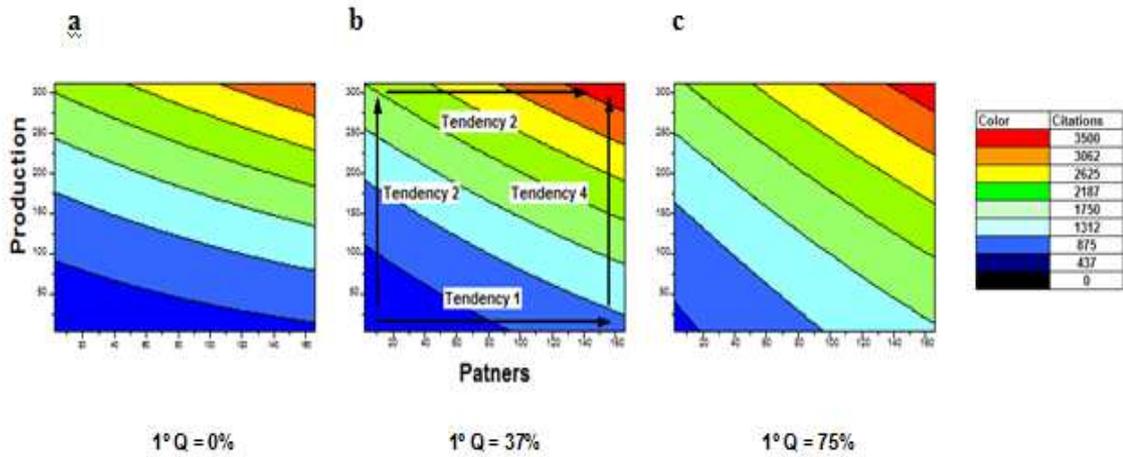


Figure 13. Surface area of the system “Scientific Community” at three levels of presence in the first quartile. Two-dimensional representation.

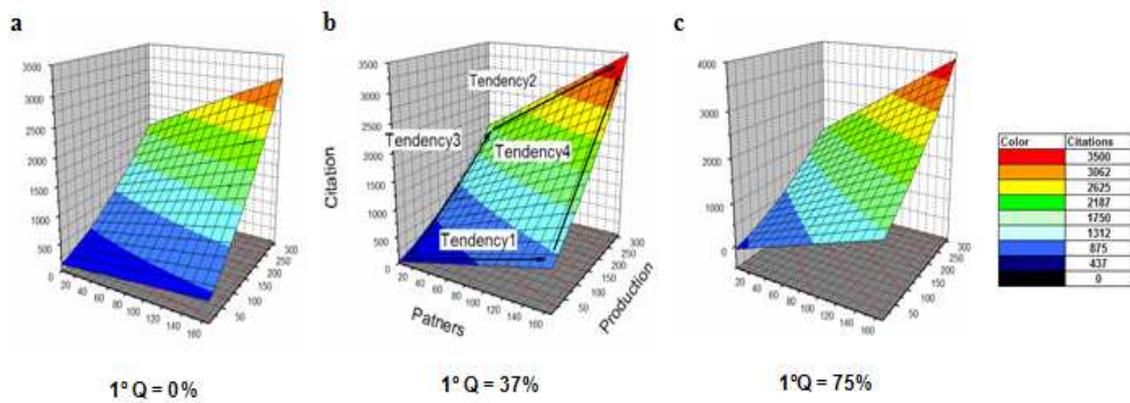


Figure 14 Response surface of the system “Scientific Community” at three levels of presence in the first quartile. Three-dimensional representation.

In the first case “the curves of level” show that, on augmenting the production of works, the number of citations also augments, until covering more than half of the trajectory of these. On the one hand, the increase in the number of co-authors also translates as an increase in the number of citations, but the response is small when only a few works are published. In

movement 1 of Figure 13, we find that the rise caused by the greater number of co-authors under low-productivity conditions does not translate as significant gains in the number of citations. Now, to reach the upper limit of the citation, it is necessary to boost significantly the number of co-authors. The increase of the production in itself is not sufficient for this; stated in other terms, from a certain threshold it is indispensable to have international co-authors to increase citations.

The situation changes decisively when a significant number of works are published in high-impact journals. Even with small production, co-authors begin to play a significantly greater role. Thus, for example, we find that low production but with a high number of co-authors offers the same results of citations expected as medium production with few co-authors (see the trajectory on the blue fringe). Similarly, average production with many international co-authors renders the same results as greater production of groups with little international participation. The highest citation is reached only in departments of groups with high production and many co-authors.

This last situation—departments that place most of their works in high-impact journals—show that the fraction corresponding to low citation is minimum. The general configuration of the sample surface shows segments arrayed in an almost perfectly diagonal way. That is, the result, measured in citations, of the groups with low collaboration and many works is the same as less productive groups but with international connections. Thus, the factor of collaboration proves absolutely determinant to reach high citation rates.

A final aspect worth highlighting is that the main differences between groups two and three is reflected above all in the lower part of the graphs. On the contrary, the behaviour in the upper fringes is very similar: the maximum citation occupies a portion and has a comparable form in the two groups, although the citation maximum value is significantly higher in the last group.

Conclusion

Regarding the methodology presented here for the first time

1. The Response Surface Method is adequate for the evaluation of scientific activity in input/output systems. They help identify causal relationships between factors and response through the construction of a mathematical model that represents the system that we have demonstrated to be robust and reliable. It also enables us to predict behaviour and locate optima.
2. Quasi-Experimental Design, the adaptation of the observational methodology of Experiment Design, enables the construction of models with only a few appropriately chosen observations. This implies a sharp decrease in the effort and cost needed to evaluate scientific activity.

Regarding the phenomena described

1. This the phenomena that we have described can be interpreted through the concept of social capital (BOURDIEU, 1998). This author defines it in this way: “Symbolic capital is an ordinary property which, perceived by social agents endowed with the categories of perception and appreciation permitting them to perceive, know and recognize it, becomes symbolically efficient, like a veritable *magical power*, a property which, because it responds to socially constituted “collective expectations” and beliefs, exercises a sort of action from a distance, without physical contact”. This capital only exists to the degree that is accepted by others, in this case the scientific community. A special kind of symbolic

capital is the scientific capital (BOURDIEU 2001) based on the recognition by others which works as a kind of credit. According to Bourdieu, the structure of the fields of Science as a whole depends on the distribution of this capital. It is interesting to observe the results of the present study in light of this conceptualization. The departments that have high scientific capital—i.e. a high capacity to relate socially to others and actively collaborate—are capable of taking better advantage of the results of the research. In our case, the scientific capital is measured in terms of the number of institutions involved in the collaboration

2. Other than we know that the impact factor (IF) of a journal does not predict the IF of an author or a particular work, what seems evident is that the prestige itself of the journal attracts citations in that we group only a certain number of works. The authors that publish in high-impact journals, which have more capacity to select from among the many works sent to them, are more visible to the scientific community, this constitutes the other determining element and closes the *virtuous* circuit of research with impact.

Now, with the general mechanics of the system established, new questions arise, so that we need to formulate questions in the future concerning the methodology of response surfaces, as for example:

- Is it only the number of individual or institutional co-authors (social/scientific capital) that increases citation? Or does it depend also on the type of collaborators?

- Does this general configuration bear details related to the nature of the research?
In our case, do clinical or basic departments render the same responses under a variation of conditions?

Surely the Response Surface Method will enable us to respond to these queries as posed above and in which the cause-effect question plays a central role.

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APPENDIX. Table A. Indicators for the Health Science Departments at the University of Navarre.

Departament	Human Resources	€ Thousands	Articles (Wos)	%1º Q (JCR-IF)	Nº Partners	Citations
ALERGOLOGIA E INMUNOLOGIA CLINICA	10	275	55	57	23	319
ANATOMIA	10	805	57	0	26	402
ANESTESIOLOGIA Y REANIMACION	30	67	16	47	3	50
AREA CARDIOVASCULAR	24	2234	170	48	59	1507
AREA NEUROCIENCIAS	42	4961	241	75	156	2939
AREA ONCOLOGIA	40	4658	195	34	132	1880
AREA TERAPIA GENICA	76	5905	240	29	143	2839
BIOLOGIA DE TUMORES CEREBRALES	6	126	7	24	15	25
BIOQUIMICA Y BIOLOGIA MOLECULAR	31	1017	118	58	94	1266
BROMATOLOGIA, TECNOLOGIA DE LOS	21	1288	85	54	32	493
CARDIOLOGIA Y CIRUGIA CARDIOVASCULAR	32	1605	202	22	129	1930
CIRUGIA GENERAL Y DIGESTIVA	13	68	65	36	13	289
CIRUGIA ORTOPEDICA Y TRAUMATOLOGIA	21	59	43	42	33	101
CIRUGIA PLASTICA, REPARADORA Y ESTETICA	9	51	31	54	6	44
DERMATOLOGIA	9	134	51	41	9	230
ENDOCRINOLOGIA Y NUTRICION	11	546	60	41	28	648
ENFERMERIA COMUNITARIA Y MATERNO INFANTIL	9	36	2	34	2	24
ENFERMERIA DE LA PERSONA ADULTA	14	13	2	38	3	8
FARMACIA CLINICA	14	12	20	52	4	94
FARMACIA Y TECNOLOGIA FARMACEUTICA	41	2241	135	64	54	855
FARMACOLOGIA	15	1506	70	22	26	565
FARMACOLOGIA CLINICA	8	119	65	28	30	270
FISIOLOGIA Y NUTRICION	30	2409	175	39	51	1166
GENETICA	14	1239	110	17	135	1074
HEMATOLOGIA Y HEMATOTERAPIA	16	1991	143	53	87	1200
HISTOLOGIA ANATOMIA PATOLOGICA	36	3144	176	42	103	1735
HUMANIDADES BIOMEDICAS	11	78	7	49	4	49
INMUNOLOGIA	7	49	40	55	30	413
INVESTIGACION Y DESARROLLO DE MEDICAMENTOS	14	29	65	39	12	193
MEDICINA INTERNA	77	6651	313	20	166	3273
MEDICINA NUCLEAR	9	805	42	48	23	273
MEDICINA PREVENTIVA Y SALUD PUBLICA	7	1175	106	41	55	801
MICROBIOLOGIA Y PARASITOLOGIA	31	1295	79	6	84	803
NEFROLOGIA	8	1174	25	43	6	93
NEUROLOGIA Y NEUROCIURUGIA	33	3025	216	25	163	3365
OFTAMOLOGIA	19	161	30	55	4	187
ONCOLOGIA	35	282	102	23	104	987
ORL Y PATOLOGIA CERVICO FACIAL	12	372	39	50	34	74
PEDIATRIA	14	257	74	38	55	259
PSIQUIATRIA Y PSICOLOGIA MEDICA	21	252	52	15	45	284
QUIMICA ORGANICA Y FARMACEUTICA	20	745	74	27	28	410
QUIMICA Y EDAFOLOGIA	40	1321	80	32	26	357
UNIDAD MORFOLOGIA E IMAGEN	5	204	30	50	24	442
UNIDAD PROTEOMICA , GENOMICA Y BIOINFORMATICA	4	214	29	12	23	122
UROLOGIA	9	14	5	67	5	67