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APPLICATION OF MATHEMATICAL MODELS IN THE KINETICS OF IN VITRO GAS PRODUCTION FOR RUMINANTS

APLICACIÓN DE MODELOS MATEMÁTICOS EN LA CINÉTICA DE PRODUCCIÓN DE GAS *IN VITRO* PARA RUMIANTES

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ABSTRACT

In vitro gas production (IVGP) is a technique that has been applied in the field of animal and agricultural production for some decades, making it the way to facilitate obtaining results without the need to harm or injure the subject in experimentation. Its results have been analyzed using different statistical-mathematical models. The purpose of this research is to highlight the application of these mathematical models that analyze the kinetics of *in vitro* gas production for ruminants. The investigation delves into linear mixed models and their different classifications, which allows them to adapt to different scientific studies. The mathematical models were also key in this research, as they form the primary structure that allows identifying what they consist of and then being able to proceed with their application. Demonstrating their usefulness in the agricultural sector was another aspect addressed, which concluded with the identification of a number of investigations carried out in recent years on the main mathematical models used to describe the kinetics of *in vitro* gas production focused on ruminants and all those elements that form a basic or supplemented food for them. Therefore, it can be said that the use of models with a mixed approach is an alternative that allows describing the kinetics of *in vitro* gas production due to the advantages they provide, making their use fundamental for the interpretation of the results.

Keywords: models, mixed linear models and agricultural sphere

Resumen

La producción de gas *in vitro* (PGIV) es una técnica que en el campo de la producción animal y agrícola se ha aplicado desde hace algunas décadas convirtiéndola en la vía que facilita la obtención de resultados sin la necesidad de dañar o lastimar al sujeto en experimentación. Sus resultados se han analizado por medio de diferentes modelos estadísticos-matemáticos. El resaltar la aplicación de esos modelos matemáticos que analizan la cinética de producción de gas *in vitro* para rumiantes es el propósito de la investigación. Se indaga en los modelos lineales mixtos y las diferentes clasificaciones que estos tienen, lo que les permite adaptarse a diferentes estudios científicos; los modelos matemáticos fueron tambien clave en esta investigación, ya que forman la estructura primaria que permite identificar en qué consisten y luego ser capaces de proceder a su aplicación. La demostración de su utilidad en la esfera agropecuaria fue otro de los aspectos tratados, que concluyó con la identificación de un número de investigaciones realizadas en los últimos años de los principales modelos matemáticos que se utilizaron para describir la cinética de producción de gas *in vitro* enfocada a los rumiantes y todos aquellos elementos que forman un alimento básico o suplementado para ellos. Por lo tanto, se puede decir que, el empleo de los modelos con enfoque mixtos resulta una alternativa que permite describir la cinética de la producción de gas *in vitro* debido a las ventajas que estos propician, siendo su uso fundamental para la interpretación de los resultados.

Palabras clave: modelos, modelos lineales mixtos y esfera agropecuaria

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Introduction

Rodríguez et al. (2017) reflect that the gas production technique is an in vitro batch system in which fermentation products accumulate. The technique is a routinely applied procedure for food evaluation and has also been used to predict voluntary food consumption in vivo (Blümmel and Becker 1997 and Blümmel et al. 1997, 2005).

In the biological field, in vitro gas production (IGP) analysis is very useful for describing the behavior of different fermentation environments. It also provides information on the composition and fermentation rates of soluble and structural constituents of foods (Rodríguez et al., 2020).

Advances in statistical-mathematical modeling allow us to reevaluate the use of classical models. The study of new approaches or alternatives to modeling phenomena can lead to more accurate results. In this regard, mixed models, combined with the analysis of critical and inflection points of functions, are powerful tools to consider in mathematical modeling in these times (García et al., 2022). In the case of IVPG, recent studies have shown that it exhibits fluctuations during the process that cannot be described by classical models to delimit its different phases.

The continuous development of research and the search for new statistical analysis strategies that provide greater precision and accuracy when obtaining results, has focused attention on determining which is the most approximate for the analysis of data from experiments with repeated measurements at different times in the same experimental unit, thus being the proposal of mixed models (Gómez et al., 2019 and Morales, 2022).

Based on the above, the present work aims to: Highlight the application of statistical-mathematical models in research on the kinetics of in vitro gas production for ruminants.

Development

Statistical-mathematical models are highly versatile tools in agricultural research. To apply the various options they offer, it is first necessary to understand what they consist of and the different models available. Linear mixed models have demonstrated efficient results in this type of study, and for this reason, we will discuss the mathematical models that have been used in recent years in agricultural research that evaluate the kinetics of in vitro gas production.

Linear Mixed Models.

The name Linear Mixed Models (MLM) according to Trilleras (2022) comes from the fact that these models are linear in the parameters and that the covariates or independent variables can involve fixed effects and random effects. Meanwhile, Altamirano et al., (2022) express that the complexity of mixed models, caused by the presence of random effects and the different covariance structures, makes the model selection process not a simple task.

This process involves repeated model adjustments and evaluations to identify a functional form that adequately describes the evolution of the response over time, its relationship to covariates, and the correlations present in the data. The use of residual-based diagnostic tools in the model-building process provides a better understanding of the problem under investigation and thus allows for the suggestion of appropriate models.

MLMs are nothing more than an extension of general linear models, whose application has been extended to studies in which it is necessary to control fixed and random effects, and measurements are made on the same experimental unit or individuals.

These models can be classified primarily based on the structure of the data and its constituent components. Navarrete (2015) states that, based on the information collected, these models can be categorized as follows:

- Fixed Effects Models: These are effects that are considered constant across the entire population. They are used to model the average effect of one or more independent variables on a dependent variable.
- Random Effects Models: These represent individual (or group) variations that cannot be explained by fixed effects. This is especially relevant in cases where the data are nested or grouped, such as in longitudinal or hierarchical studies.
- Multilevel or Hierarchical Models: These are applied when the data have a hierarchical structure, that is, the observations are grouped at different levels (for example, students within schools) and the aim is to model variability across these levels.
- Repeated Measures Models: Used when the same observations are taken multiple times over time or under different conditions, allowing analyses to account for correlation between observations within the same subjects.
- Longitudinal Models: These focus on changes over time involving the same subjects, allowing for analysis of how certain effects vary over a long period.
- Univariate Models: They address a single continuous response in the analysis.
- Multivariate Models: Allow for the evaluation of multiple dependent variables at once, facilitating a more complex analysis that includes the interdependencies between different responses.

Mathematical Models

A mathematical model is a simplified representation, using mathematical equations, functions, or formulas, of the relationship between two or more variables. On the other hand, the branch of mathematics that studies the qualities and structure of models is known as "model theory" (Roldán, 2019).

According to Ramos in 2021, mathematical models can be classified according to the outcome they predict: deterministic and stochastic models. The former predict the same outcome in their measurements because they start from a specific perspective; this is because they ignore random variation. The latter predict the distribution of possible outcomes, as they are more statistical in nature.

When defining a mathematical model, it is necessary to understand that it is made up of the interrelation of formulas, letters and numbers that, when combined, achieve an efficient expression, capable of describing and relating those parameters or values where its use is necessary.

According to Roldán (2019), many of these types of mathematical models can also be classified according to the information they represent:

- According to the information used
  - Heuristic: Based on possible explanations for the causes of observed phenomena.
  - Empirical: Uses information from real experimentation.
- By type of representation
  - Qualitative or conceptual: They refer to an analysis of the quality or trend of a phenomenon without calculating an exact value.
  - Quantitative or numerical: The results obtained have a specific value that has a certain meaning (it can be exact or relative).
- According to randomness
  - Deterministic: There is no uncertainty, the values are known.
  - Stochastic: The exact value of the variables is not known at all times. There is uncertainty, and therefore a probability distribution of the outcomes.
- Depending on your application or objective
  - Simulation or descriptive: Simulates or describes a phenomenon. The results focus on predicting what will happen in a given situation.
  - Optimization: They are used to find an optimal solution to a problem.
  - Control: To maintain control of an organization or system and determine the variables that must be adjusted to obtain the desired results.

The selection of the mathematical model cannot proceed without first defining its statistical selection criteria. Telles et al., 2018, noted that the selection of the best model is based on goodness of fit, measured by the sum of squares of the error (SSE), the root mean square error (RMSE), the coefficient of determination adjusted by the number of model parameters (R^2adj), and the significance of the parameters.

Use of mathematical models in agricultural sciences

In agricultural sciences, various models have been used to predict the behavior of various research projects due to their usefulness. Rodríguez et al. (2018) compiled a collection of studies using mathematical statistical models in agricultural sciences and found, in some of them, models that compare the response to measuring nitrogen doses in corn and coffee. Using the modeling results, they were able to recommend the optimal dose of nitrogen fertilizers for these crops.

Telles et al., (2018) carried out a study to predict the stem volume of Tectona grandis L. f. in an 11-year-old plantation in Nuevo Urecho, Michoacán, in which after adjusting six stem volume models through the goodness-of-fit selection criteria, the Meyer model was the appropriate one to most accurately predict stem volume based on the normal diameter (d) and total height (AT) of T. grandis in plantations with physical and biological conditions similar to those of the site of this study.

Sobalvarro et al., (2019) manage to apply mathematical models with the purpose of determining the behavior of in vitro gas production from concentrates of star grass (Cynodon nlemfuensis), ryegrass (Lolium perenne), mulberry (Morus alba), corn silage (Zea mays) and concentrated feed incubated with ruminal liquor to estimate the net lactation energy in cattle.

Duran et al., (2022) reflect in their article the use of simulation models applied to phytosanitary, especially in crops associated with pests and diseases, demonstrating that these are increasing over time since the variables are related: climate elements, growth and development of the crop, as well as the behavior of pests and diseases, agreeing that these are topics in which modeling plays a significant role in the sample of results.

Statistical models most widely used to describe the kinetics of in vitro gas production

In recent decades, the use of nonlinear models to describe the behavior of in vitro gas production kinetics has become frequent, among which the Logistic, Gompertz, among others, are most widely applied. However, it has currently been shown that their application is not the most appropriate when measurements are made on the same experimental unit, so it is necessary to search for other models for better interpretation. According to García et al., (2022), a frequent problem when modeling this type of data is that the residuals are correlated with each other, being one of the main causes in in vitro gas production since measurements are made over time on the same experimental unit, which is why a specific variance structure is generated.

Given this situation, nonlinear mixed models (NLMs) are an alternative approach. They can be used to model the correlation structure, either directly or using random variables. Other advantages of the mixed approach include that it does not require the data to be normally distributed, helps control heterogeneity, improves statistical fit criteria, and has positive effects on the analysis of NLMs, fitted to longitudinal data according to Gómez and Agüero in 2020.

Bandera and Pérez (2018) point out that mixed models gain value in the agricultural field because they are applied in the analysis of longitudinal data, multi-environment trials, and growth curves. Furthermore, Gómez et al. (2019) suggest that the use of linear models with a mixed approach is common in the analysis of variance of in vitro gas production experiments with repeated measures.

Torres et al. (2018) used the Gompertz model to evaluate the gas production and in vitro degradability of white oak (Quercus spp.) leaves included in feedlot calf diets. They obtained significant results for reducing the in vitro production of ammoniacal nitrogen when including oak leaves, as well as the constant rate of gas and methane production.

Sequen (2022) carried out a study to determine the in vitro ruminal disappearance of the soluble fraction of mulberry (Morus alba) leaves, where he used the exponential model to obtain gas production up to 24 hours of incubation. This same author carried out a second modeling to understand the degradation of the dry matter of the soluble fraction of mulberry hay, and it was the Gompertz model that best described the degradation of the easily degradable portions.

According to da Silva et al., (2021), mathematical models are used to describe biological phenomena, and in animal nutrition they are used to adjust in vitro gas production. Authors such as Morales (2023) used the Gompertz model to evaluate biogas and methane production in samples of carob (Samanea saman (Jacq.) Merr.) and parota (Enterolobium cyclocarpum (Jacq) Griseb.) pods as a feed supplement in cattle.

García et al. (2022) evaluated classical models (Gompertz and Logistic) and alternative models with the addition of a trigonometric function to these models, to describe the in vitro gas production kinetics of ruminant feeds. The authors found that the extended models had an adequate fit and fulfilled the assumptions, with the extended Gompertz being the most comprehensive for describing said kinetics.

Conclusions

1. Linear mixed models are basic tools for carrying out the application of modeling in different research projects.
2. Mathematical models have a strong influence in the agricultural sector; their use in research on in vitro gas production facilitates the identification and description of production kinetics.
3. Gompertz and Logistic mathematical models are the most detailed models of in vitro gas production kinetics when evaluating experiments with animals (mainly ruminants) and pastures. They are an effective alternative for interpreting results.

References

Altamirano, M., Rapelli, C. M., y Catalano, M. (2022). Técnicas gráficas de diagnóstico para los modelos lineales mixtos.

Bandera, E., y Pérez, L. (2018). Los modelos lineales generalizados mixtos. Su aplicación en el mejoramiento de plantas. Rev. Cultivos Tropicales, 39(1):127-133. Ministerio de Educación Superior. Cuba.

Blümmel, M. y Becker, K. (1997). "The degradability characteristics of fifty-four roughages and roughage neutral-detergent fibers as described by *in vitro* gas production and their relationship to voluntary feed intake". British Journal of Nutrition, 77(5): 757-768, ISSN: 1475-2662, 0007-1145, https://doi.org/10.1079/BJN19970073

Blümmel, M., Cone, J. W., Van, A. H., Nshalai, I., Umunna, N. N., Makkar, H. P. S. y Becker, K. (2005). "Prediction of forage intake using *in vitro* gas production methods: Comparison of multiphase fermentation kinetics measured in an automated gas test, and combined gas volume and substrate degradability measurements in a manual syringe system". Animal Feed Science and Technology, 123-124(Part 1): 517-526, ISSN: 0377-8401, https://doi.org/10.1016/j.anifeedsci.2005.04.040

Blümmel, M., Steinga, H. y Becker, K. (1997). "The relationship between *in vitro* gas production, *in vitro* microbial biomass yield and 15N incorporation and its implications for the prediction of voluntary feed intake of roughages". British Journal of Nutrition, 77(6): 911-921, ISSN: 1475-2662, 0007-1145, https://doi.org/10.1079/BJN19970089

da Silva, C.Z., Ítavo, L. C.V., Ítavo, C. C.B. F., dos Santos, G. T., Dias, A.M., dos Santos, G., y Gurgel, A. L. C. (2021). Kinetics of *in vitro* gas production and fitting mathematical models of corn silage. Fermentation, 7(4), 298

Duran, E., Acuayte, E., Acuayte, M. C., Hernández, J. C, y López, I. L. (2022). La modelación y simulación matemáticas: una herramienta para la protección de cultivos. Revista Mexicana de Ciencias Agrícolas, 13(6), 1129-1140. Disponible en: https://doi.org/10.29312/remexca.v13i6.2922

García, Y., Herrera, M., Rodríguez, R., y Ontivero, Y. (2022). Evaluation of non-linear and mixed non-linear models to describe *in vitro* gas production kinetics of ruminant feeds. Cuban Journal of Agricultural Science, 56(1).

Gómez, S., Torres, V., García, Y., Herrera, M., Medina, Y. y Rodríguez, R. (2019). "Procedimiento estadístico para el análisis de experimentos con medidas repetidas en el tiempo en la esfera agropecuaria". Cuba. J. Agric. Sci. 53(4): 353-360, ISSN: 2079-3480.

Morales, A. F. (2022). Estudio comparativo de los métodos de diagnóstico para modelos lineales mixtos y modelos lineales generalizados. Tesis de Maestría. Colombia

Morales, B. K. (2023). Evaluación de dos vainas de leguminosas arbóreas como estrategia en la producción bovina tropical. (Tesis de Maestría). Guerrero, México.

Navarrete, O. V. (2015). Análisis comparativo de modelos de respuesta al ítem explicativo. Tesis de Maestría. Guayaquil, Ecuador. https://www.dspace.espol.edu.ec/retrieve/b7635b72-2604-404a-afdb-169ccfbba9e8/D-CD71899.pdf

Rodríguez, O., Florido, R y Varela, M. 2018. Aplicaciones de la modelación matemática y la simulación de cultivos agrícolas en Cuba. Rev Cultivos Tropicales, 39(1):121-126.

Rodríguez, R., Galindo, J. L., Iraola, J., y Gómez, S. (2017). Uso de la técnica de producción de gas para predecir la relación entre el nivel de consumo e indicadores de la fermentación ruminal *in vitro*. Cuban J. Agric. Sci. [online]. 51(3):301-310. ISSN 2079-3480. http://scielo.sld.cu/scielo.php?script=sci_arttext&pid=S2079-34802017000300003&lng=es&nrm=iso

Rodríguez, R., Ontivero, Y., García, Y., Sosa, D. y Gómez, S. (2020). Empleo del tubérculo de boniato *(Ipomoea batatas L.*) y la cepa *Lactobacillus pentosus* LB-31 como aditivos a ensilajes mixtos para rumiantes. Livestock Research for Rural Development. 32(117), ISSN: 0121-3784, DOI: http://www.lrrd.org/lrrd32/7/rodri32117.html

Roldán, P.N. (2019). Modelo matemático: Qué es, para qué sirve y tipos. Economipedia.com Disponible en: https://economipedia.com/definiciones/modelo-matematico.html

Sequen, C. E. (2022). Determinación de la desaparición ruminal *in vitro* de la fracción soluble de hoja de morera (*Morus alba*) (Doctoral dissertation, Universidad de San Carlos de Guatemala)

Sobalvarro, J. L., Elizondo, J. A. y Rojas, A. (2019). La producción de gas *in vitro* para estimar la energía neta de lactancia. Rev AAgronomía Mesoamericana, 31(2):311-328. Costa Rica. https://doi.org/10.15517/am.v3li2.38497

Telles, R., Gómez, M., Alanís, E., Aguirre, O. A y Jiménez, J. (2018). Selection and adjustment of mathematical models to predict the stem volume of Tectona grandis L. f. in Nuevo Urecho, Michoacan, Mexico. Rev Madera y Bosques, 24(3). https://doi.org/10.21829/myb.2018.2431544

Trilleras, M. (2022). Implementación de modelos lineales mixtos flexibles a datos de crecimiento craneofacial en la cohorte CESLPH-Damasco. Tesis de Maestría. Medellín, Colombia