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Algorithms and Tools for Analysing and Planning Experiments in the Agro-Industrial Complex

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Abstract. The paper examines the application of systematic and risk-based approaches to problem solving in the agro-industrial complex, which generally prompted research in the field of various model-based methodologies. Of particular interest to this study is the Quality by Design initiative in the agro-industrial complex. Motivated by their need, this paper reports some of the contributions to analysing the existence and availability of the experimental plan. The analysis of the feasibility and adaptation of the nested sampling algorithm for the probabilistic characteristics of the design space is considered. There is described an initial adaptation of the nested sampling algorithm, common for large Bayesian calculations, for the probabilistic characterization of spatial design, which is a key work for practitioners in the agro-industrial complex. The choice-based approach has been found to be effective with the optimization approach, allowing practitioners to take advantage of the choice-based approach with other methods. A step-by-step technology is given for complex and one-time implementations of the original nested sample for spatial design, which further reduces the computational load, thereby allowing solutions of more complex problems. Design-centring methodology is shown as an alternative coding method for methodological choice, providing the practitioner with a convenient format for communicating with process operators. A particular attention is paid to several pronounced problems that arise in the special design of experiments when there are various levels of model uncertainty, which are often encountered in the early stages of model development. The paper presents the results of the study obtained by developing optimal experimental queries in the presence of restrictions.

INTRODUCTION

This research study assesses several special cases as follows: how best to collect and use scientific knowledge encoded in the form of a mathematical model, with an emphasis on the treatment of uncertainty. Special cases are motivated by important problems of modern engineering of technological systems in relation to the agro-industrial complex for a better understanding of the impact of climate change [1–16]. The agro-industrial complex plays a crucial role in attaining the Sustainable Development Goals [17–26] within ending poverty by creating job opportunities and improving the incomes of farmers and other stakeholders [27–35]. The agro-industrial complex can help small farmers and agro-entrepreneurs increase their productivity and profitability by providing access to markets, financing, and technology [36–42]. In addition, it contributes to sustainable food systems by promoting sustainable agriculture, reducing food waste and loss, and promoting the consumption of healthy and nutritious diets [43–52]. By adopting sustainable practices such as agroforestry and conservation agriculture, the agro-industrial complex can also help reduce greenhouse gas emissions and mitigate climate change [53–61]. It contributes to economic growth by

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promoting sustainable agribusiness and agro-processing. By creating job opportunities and promoting value addition, it helps increase the incomes of farmers and other stakeholders in the agricultural value chain. The agro-industrial complex can promote innovation in agriculture by adopting new technologies and practices.

The quality-by-design initiative promotes a scientific and risk-based approach to the development and production of agricultural products. The initiative introduces a new range of activities for farmers, leading to the widespread adoption of technology system tools and methods that use mechanistic process models. The overall goal of this study is to develop methodologies and technology systems tools to support the initiative. To achieve this, the following goals are set:

- Improve the computational efficiency of sample-based methodologies for characterizing the design space and provide efficient methods for their use.
- Develop new methods for the optimal design of the experiment, focusing on the optimal calibration of nonlinear models in the early stages of their development.
- Demonstrate new methodologies for research in the agro-industrial complex.
- Implement software to further promote the use of the developed methodologies.

MODEL ALGORITHM AND EXPERIMENTAL DESIGN

Enterprises need to solve their problems quickly and efficiently [62–75]. In this context, systematic and integrated methods require the equally efficient and rapid development of mechanistic modelling. A simplified version of one of the most widely used frameworks for mechanistic modelling highlights two key phases in which a careful design of experiments plays a crucial role: separation and calibration. The process begins with a set of preliminary experiments and measurements of the system of interest, which may be based on scientific data, documents, laws, or practical experiences acquired by the experimenter within the system. Researchers initiate this process by proposing potential model structures that can explain the system, often considering several alternative and competing models. When a single model can be identified as the most suitable, the experimenter proceeds to the calibration phase.

There are two approaches to addressing multiple competing models. The first is to decide that it is not necessary to determine the most suitable model. Forecasts are made using the Bayesian model averaging method [76], in which expectations are obtained from model forecasts weighted by their likelihood. An alternative approach is to determine the most appropriate construct before proceeding to the calibration stage [77]. Experiments are conducted to refine and improve the accuracy of the model parameters until the required accuracy is reached. The appropriate level of accuracy should be determined by the end goal of the simulation and will often depend on the specific situation.

The term "model-based planning of experiments" was coined by the Society of Process Systems Engineers [78] to denote a set of methods for planning experiments that complement the development of mechanistic models. The term "model-based" refers to the fact that mathematical models are used to create optimal experimental designs. An important feature of planning experiments based on models is the interdependence between the experimental plan and the model itself. The purpose of experiments is to create the model as efficiently and quickly as possible, but their effectiveness also depends on the accuracy of the model. Although this feature creates difficulties when planning experiments based on models, it is simply a natural and inevitable consequence of the learning process. However, a model that may be imperfect at the time represents the experimenter's best understanding of the existing system. Of particular note are mechanistic models that contain physical data that can be invaluable when conducting experiments. After one measurement is made, the experimenter's understanding changes, as does the model. Therefore, the optimal experimental campaign often changes as more data are collected. Ideally, campaigns are updated immediately after collecting any measurements so that they use all available information as it becomes available. However, this feature is limited by the refresh rate of experimental campaigns. In addition, this choice depends on whether the campaigns run in parallel or at the same time.

RESULTS OF CALIBRATION

One of the main reasons why thinking about planning experiments when developing a model is fruitful is the uncertain nature of reality. In the absence of uncertainty, it would be easy to develop a model and experiment. However, the reality is that no matter how well the experimenter plans and executes the experiment, random errors will break the relationship between the input and output of the system. Optimal calibration experiments address this problem by deliberately choosing input values to minimize the impact of random errors on the uncertainty of the model parameters.

Although experimentation is at the heart of the scientific method, the first well-documented contribution to the optimal design of an experiment was made more recently in a paper [79]. A paper three decades ahead of its time obtained G-optimal experiments for one-dimensional polynomials up to six. Smith's paper does not seem to have been directly influential, followed by [80], which many consider to be the seminal work on planning experiments. It begins by presenting the principles of well-planned experiments through a tea-tasting experiment. This is a qualitative example if the question is to evaluate a woman's claim that she can determine what is added first – tea or milk when making tea – by trying it. In the following chapters, examples of agricultural experiments are presented, the purpose of which is to determine the relative productivity of different crops. Without formally addressing the issue, the book argues that it is optimal to divide the experimental area of the Earth (roughly rectangular) in the form of a Latin square. For example, with 5 cultivars named *A, B, C, D,* and *E*, the experimenter should divide the experimental area into 5 × 5 plots and arrange the cultivars as follows:

$$\begin{matrix} A & B & C & D & E \\ E & A & B & C & D \\ D & E & A & B & C \\ C & D & E & A & B \\ B & C & D & E & A \end{matrix}$$

Each variety appears exactly once in each row and column. Later, the Latin square d-scheme was proven to be optimal in a seminal paper [81], who also proposed maximizing the determinant of the information matrix as a measure of experimental information.

In the next two decades, the development of basic theories of optimal planning of experiments accelerated. The scholar [82] defined the relationship between the d-optimal criterion and Shannon's concept of entropy [83], adopting the Bayesian concept of statistics. The study [84] aimed to investigate the C-optimal and A-optimal measurements for a two-parameter two-factor regression model with two parameters θ1x1 + θ2x2, where θ1 and θ2 are model parameters and x1 and x2 are experimental controls. In the same paper, Elfving presented a basic geometric interpretation of the C- and A-optimal criteria, which was later extended by [85] to all alphabetic criteria, eventually leading to the Elfving set [86]. Two review papers by [87] and [88] provide clear insight into the contribution of Elfwing to optimal experimental design. The study [84] appears to be the first documented publication to present the concept of support with optimal experimental design. These optimal campaigns are repeats of a recent and often small number of unique experiments. Furthermore, based on [87] review, Elfving may have been the first to apply Caratheodory's theorem to experimental planning, proving that for all optimal experimental planning problems, there exists an optimal campaign of no more than nθ(nθ + 1)/2. number of supports, where nθ is the number of model parameters. A year later, [89] extended [84] to consider nonlinear models, thus introducing the basic method of local design and coining the term locally optimal plans. Jack Kiefer is cited by [90] and [91] as a key contributor to the development of the basic theory of experimental design. An alphabetical naming system for the various information criteria used in an experiment.

The design literature was presented by [92]. The researcher [93] followed [94], derived optimal plans G and D for univariate multinomial regression models and derived alternative plans. Their work proved the equivalence of d-optimality and G-optimality [95]. As [91] notes, [95] also establishes a "continuous" or "approximate" theory of experimental designs in which the computational difficulties associated with the number of experimental launches are eliminated. Continuity theory led to Kiefer's famous General Equivalence Theorem [96]. The General Equivalence Theorem helped solve the problems of planning experiments, which led to the development of algorithms for calculating optimal plans of experiments. First-order algorithms are a class of algorithms using the general equivalence theorem (see chapters 3.1 and 3.2 of [90]), also called peak rise or fall (see section 9.4 of [97]).

Applications of the optimal design of experiments go hand in hand with many early theoretical developments. The paper [98] is one of the first applications to the determination of optimal experimental designs involving multiple experimental factors, with emphasis on the calibration of planned regression models. The paper first introduced the concept of rotational optimal design, which was first developed [99]. Study [100] is one of the first applications of the optimal design of an experiment to a transient or dynamic system in which the state variables change over time. They described how to calculate optimal plans for three nonlinear models of local D-chemical kinetics, choose optimal sampling periods for a periodic experiment – the time at which product release is observed, and consider additional experimental factors such as initial concentration and temperature. In addition, the document introduces the concept of "design locus" to provide geometrical interpretation of local d-optimal plans along with actual drawings of the Concept.

An obstacle to the widespread implementation of optimal design of experiments for nonlinear models is the dependence of optimal experiments on unknown parameters of the model. Following [89] basic technique of local design, there have been several major changes. A conference by [101] first proposed the idea of using sequential experiments for nonlinear models, where experiments are performed one at a time and model parameters are updated between experiments. The example discussed was a single response model for chemical kinetics with three model parameters for the reaction R → P + P1, where r is the reactant (starting alcohol), p is the desired product (olefin), and *P1* is the byproduct (water). Starting with a 22-factor design to obtain an initial estimate of the model parameters, they calculated 9 more runs one at a time, updating the values of the model parameters at each new response measure. The scholar [102] was the first to propose the use of Bayesian and maximin plots to calibrate nonlinear models. These criteria are later applied - under the names expected value and worst-case approach (respectively) - to dynamical systems [103] and [104]. Despite its early use [100], [105] and [78], the application of experimental design theory to dynamic systems has been relatively slow compared to its introduction to stationary systems.

The study [105] suggests that one reason is the limited exposure of dynamic systems modellers to the extensive literature on experimental design. A paper [106] presented a rigorous and convenient methodology for the application of design-of-experiment theory, which has been incorporated several times over time. Control vector parameterization is used to approximate time-varying inputs in the form of control profiles. They calculated optimal experiments for model recognition and optimal calibration. In the study [77], the criterion was used to distinguish models. However, it should be noted that an unconventional criterion that maximizes the amount of sensitivity of the measured responses to the model parameters is used to calculate and possibly control the optimal calibration experiment. The first concept of the sequential design of nonlinear models was developed [107]. They present a nontraditional method that takes advantage of the availability of frequent measurements in dynamic experiments with time-varying experimental factors. This method involves reconstructing the experiments as they are performed, which requires online updating of the experimental model and design each time a dynamic experiment is performed. Application of this method requires a fast and reliable way to estimate the parameters of the model and experimental design.

When planning experiments of experimental applications, there are cases where the experimenter cannot precisely control the values of the experimental factors. An obvious example of this is animal husbandry, perhaps when blood samples can be taken from animals. Reference [108] presented a method for designing optimal windows or sampling intervals. This method was later used [109] to support pharmacokinetic modelling and obtain efficient optimal selection windows to increase flexibility and feasibility in clinical practice.

Another important area of optimal calibration research is to reduce the correlation between parameter estimates. One of the earliest published works on this topic is [110]. More recently, a previous study [111] emphasized the importance of correlation in optimal experimental calibration designs and proposed several suitable criteria for experimental designs. They described design procedures in which correlation-based criteria are included as additional objectives or constraints to the optimization task.

This motivated a later contribution [112], in which a two-objective framework is proposed to compute a group of efficient plans that minimizes correlation and increases parameter accuracy. We have highlighted several key contributions to methods beyond the classical theory of optimal experimental planning. A previous study [113] suggested developing a methodology of dynamic experiments to optimize dynamic processes in the absence of a mechanical model. This method is used in the studies [114] and [115] to better represent the nonlinear behavior of dynamical processes by introducing an exponential time transformation and improved in the study [116], where regression constraints are introduced based on a mechanistic understanding of the system to significantly improve model fit. An experiment planning method to optimally calibrate an approximate model where the model is known not to fit the desired region. This method can be described on the basis of an initial set of experimental data. A model-based data mining technique is used instead of conventional parameter estimation exercises to classify raw data as model-fit or not-fit and to derive an initial set of parameter estimates using only compatible data. A supervised phase of machine learning is then used to predict the domain of action or compatibility. A standard measure of optimal calibration is then used to plan the experiment within the confidence region [117–122].

DISCUSSION OF ANALYSIS FEASIBILITY, STABILITY AND FLEXIBILITY

This section focuses on fundamental developments in the field of flexibility analysis, particularly in the process systems engineering literature. The development of flexibility analysis begins with the problem of designing processes. It involves determining the values of design variables that remain constant and unchanged throughout the life cycle of the process. In many cases, they are related to the design of the equipment, for example, the size of the equipment. However, in an agro-industrial complex, operational variables such as batch time can be considered as design variables, as rules may limit the change in their values. During design, it is necessary to consider the various constraints that determine the feasibility of the process, as well as the presence of uncertainties, which can be divided into external and internal uncertainties. Examples of the former include water temperature, process feedstock composition or demand, and seed market price. Examples of the latter include the order of various substances, heat and mass transfer coefficients or fugacity coefficients. An important aspect of these uncertainties is the time scale over which they operate. For example, consider the comparison between sudden changes in market prices of products that can be caused by supply chain failures and gradual water temperature cycles due to the seasons. The main difference between intrinsic and extrinsic uncertainties in terms of experimental design is that deliberate and rational experimentation can reduce intrinsic uncertainties. In contrast, little (or nothing) can be done to reduce external uncertainties, so methodologies are needed to make robust decisions against them.

Feasibility, stability and flexibility analysis is a set of quantitative methods used in the development and operation of processes under uncertainty. A more rigorous formulation of the enterprise design problem is called design under uncertainty. Due to the complexity of stating the max-min-max constraints, several concessions have been introduced that allow us to use production-critical examples in minutes.

Design methods for sustainable processes have been developed. Then, parallel developments in the field of stability and flexibility were formalized and included in the work. Flexibility refers to the degree to which a process can perform under changing conditions, while fault tolerance measures the dynamic ability of the process to recover from disruptions. In particular, fault tolerance takes into account how fast and smooth the recovery trajectory is.

The methods are further classified as analysis methods and design methods. The only difference is that the former applies to a fixed scheme of process d, while the latter aims to determine the optimal scheme d. As the field has developed, two problems have come to dominate elasticity analysis: elasticity test problems and elasticity index problems. The solution of the first determines whether a scheme of a certain process is possible within a certain range of uncertainty. The latter aims at quantifying the largest ranges of uncertainty (in scalar form) for the design of this process.

For this work, of particular interest is the quantification of elasticity using the concept of stochastic elasticity. In such a probabilistic framework, process flexibility is quantified as the likelihood that the project will lead to a feasible operation. The main obstacle to the implementation of these methods is an efficient solution methodology. Random constraint programming is a set of techniques suitable for the analysis and design of stochastic flexibility.

A component of process flexibility is the presence of regression operations to reduce the uncertainties of the process being measured. Some of the process uncertainties can be measured, which makes it possible to eliminate their uncertainty by measurement. When measurements of process disturbances can be made quickly and frequently, corrective actions can be implemented to mitigate adverse process responses caused by these disturbances. Although these comments are optional, they are considered important in the process control systems community.

CONCLUSION

Agro-Industrial Complex plays a vital role in attaining the Sustainable Development Goals by promoting sustainable agriculture, reducing poverty, improving food security and nutrition, promoting clean water and sanitation, and contributing to economic growth [123–135] and innovation [136–153]. Financial institutions play a critical role in providing credit and other financial services to farmers, agro-entrepreneurs, and other stakeholders in the agricultural value chain. Financial institutions can also support the development of the agro-industrial complex by investing in agribusinesses and other related industries [154–163]. This, in turn, can contribute to economic development, job creation, and poverty reduction, which are essential components of sustainable development [164–170]. It should be noted that education [171–186] can also help to promote innovation and technology transfer in the agro-industrial complex, which is essential for improving productivity, efficiency, and competitiveness. Energy efficiency impacts reducing the cost of production, increasing productivity, and reducing greenhouse gas emissions in agro-industrial complexes with developing innovation technologies [187–194].

This paper discussed the development of new algorithms and tools for experimental feasibility analysis and optimal planning. Successful adoption of the nested sampling algorithm has also been reported, which provides farmers with an efficient sampling method to characterize a probabilistic design space suitable for solving large-scale problems. For the design space, the nested sampling method draws point samples with a gradual increase in density to the desired level of confidence, which is greatly improved by the base Monte Carlo model and the final method based on competitive optimization. The key to this efficiency is the design of the chosen replacement offer. The ellipsoid that was expanded was effective around the current live points. Further improvements made it possible to increase the efficiency of the method, showing a reduction in the total calculation time by 4-5 times for an industrially important example. Applying the results of sample-based methods requires converting the samples into a format that can be used by experienced farmers or veterinarians.

Additionally, the paper is devoted to the creation of an optimal experimental design. Many applications of optimal experimental planning in agricultural engineering ignore the basic concept of experimental support and effort. In an attempt to reintroduce such concepts, a methodology is proposed that uses these concepts and demonstrates their suitability for creating real dynamic experimental campaigns. This approach brought additional advantages, including an increased optimization problem and a completely independent computational step before optimization that could be parallelized to reduce computational time if needed. An optimal experimental design is useful in the early stages of model development when large modelling uncertainties prevail. The two-objective framework solves the problem of suboptimal experiments due to imprecise values of model parameters. The problem of planning probabilistic experiments with significant modelling uncertainties is framed within the probabilistic paradigm. A major contribution was the integration of a continuous force design method and method into a two-step computational framework. The strengths and synergistic advantages of the two methods made it possible to solve the real problem of optimal experimental planning, which, according to the authors, was not available at the time.

Despite extensive use of experimental feasibility analysis and optimal planning, there has been no reliable, flexible implementation of either open source method. This deficiency can hinder many potential applications.

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