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Optimal Design Strategies for Toxicological Tests

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Abstract

A lot of toxicological testing is done to learn about toxicity in aquatic environments. This kind of experiment, whose response variable is determined by counts, may have reproduction as one of its endpoints. There is research on the best probability distribution to utilise for the data analysis. The assumption of this probability distribution is crucial to the theory of optimum experimental design, and when it is incorrect, the produced design may be less efficient. The major goal of this work is to suggest reliable designs when the probability distribution of the response variable is unknown. In order to accomplish this, three distinct approaches are introduced, contrasted, and then used in toxicological testing based on Ceriodaphnia dubia.

Keywords: D-optimality; An exponential family; An information matrix; Distribution logical linear mode

Introduction

Toxicological assays are a fundamental and frequently-used method for analysing the effects of chemicals in aquatic environments and determining the safe amounts at which these chemicals will not impair the development of aquatic species [1]. Reproduction is a frequent endpoint in these studies as it tells us about the population dynamics of the species in the ecosystem. Thus, in the presence of various concentrations of the studied chemical, these tests evaluate evolution in the reproduction of the species [2].

Techniques created in the area of optimal experimental design are highly beneficial in this type of controlled experiment. The goal of the theory of optimum experimental design is to pinpoint the ideal conditions in which an experiment should be conducted in order to maximise the knowledge that will be gleaned from it. In order to describe the study that was conducted, this information is later employed in the data analysis. In order to conserve resources and produce high-quality data, it is crucial to have the ability to properly plan the experiments for these toxicological testing. Although there are many studies that examine the results from this kind of experiment, there is a dearth of literature on the best experimental design to use for toxicological tests that is only relevant to hormesis. Using Caseros-Alonso et al research [3, 4,5].

Strategies for obtaining robust designs

Pozuelo-Campos et al. demonstrate the significance that the assumption of the probability distribution and the response variable may have for optimal experimental design and its impact on the predicted design efficiency in case of misspecification. This paper suggests many methods for developing robust designs that enable the impact of the error to be reduced while taking into account the existence of uncertainty while assuming a probability distribution. The three proposed solutions are given a general overview in this part, and their behaviour and effectiveness are then examined by applying them to toxicological testing.

In the literature on the best experimental design, the compounding of criteria is a frequently used approach. The use of the compound criterion enables the researcher to generate a design that simultaneously considers two distinct objectives defined as two optimization criteria, 1 and 2, weighted in accordance with the researcher's needs. Thus, this criterion is established. In the context of this study, the absence of prior knowledge about the experiment is typically the cause of uncertainty in the probability distribution of the response variable. A multistage experiment, is one alternative to take into account. Using the data, this experimentation technique involves segmenting all of the available observations into discrete stages [6].

Starting with a random initial design, the procedure is said to contain m (m + 1)/2 + 1 points in its support, which is the maximum allowed by Caratheodory's Theorem. This initial design is then repeatedly perturbed; either at one point or one weight every iteration, a predetermined number of times selected by the user. These perturbations get smaller as the process goes on. It should be observed that when one of the weights is disturbed, the other weights are adjusted so that they continue to satisfy the requirement that their combined amount be one. Some weights may converge to zero as the algorithm continues to run. The method reduces the amount of the perturbations after each run, with a pre-determined minimum amplitude serving as the halting condition [7, 8].

The probability distribution of the response variable is unclear when the reproduction is used as the endpoint, as demonstrated in Section 1, and this uncertainty might affect how effectively the best design is implemented. The best designs for the aforementioned toxicological tests are first determined in this section for each probability distribution individually. The techniques are then used to create sturdy designs. In order to identify the behaviour of the parameter estimators, a simulation study is conducted in the end. There is literature that discusses the probability distribution to be taken into account for the results obtained in toxicological experiments when the reproduction of a species is the endpoint. Keeping in mind the tests covered in this paper. Similar to Pozuelo-Campos, a variance structure resembling the Poisson distribution is taken into account while analysing the heteroscedastic normal distribution [9, 10].

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Declaration of competing interest

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