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Nonparametric Bayesian Optimal Designs for Exponential Regression Model with Polya Urn Scheme as the Base Measure

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Abstract
This study introduces optimal designs for the Exponential nonlinear model using nonparametric Bayesian approaches. Nonlinear regression models find extensive applications across various scientific disciplines. It is vital to accurately fit the optimal nonlinear model while considering the biases of the Bayesian optimal design. By utilizing the Dirichlet process as a prior, we present a Bayesian optimal design. In this research paper, we employ a representation to approximate the D-optimality criterion considering the Dirichlet process as a functional tool. Through this approach, we aim to identify a Nonparametric Bayesian optimal design.

Keywords: D-optimal design, Bayesian optimal design, Unit Exponential model, information matrix, Dirichlet process, Nonparametric Bayesian.

Introduction

As discussed in our previous work (Nanvapisheh et al., 2023; Nanvapisheh , et al., 2024; Nanvapisheh et al., 2024), in experimental design, the term "optimal design" refers to a specific class of designs categorized according to particular statistical criteria. It is widely acknowledged that a well-designed experiment can significantly enhance the accuracy of statistical analyses, specifically the accuracy of the parameters corresponding to the size of the parametric confidence region. Consequently, numerous researchers have dedicated their efforts to address the challenge of constructing optimal designs for nonlinear regression models. Experimental design plays a pivotal role in scientific research domains, including but not limited to biomedicine and pharmacokinetics. Its application in these fields enables researchers to conduct rigorous investigations and yield valuable insights.

Optimal designs are sought using optimality criteria, typically based on the information matrix. In nonlinear models, the presence of unknown parameters introduced complexities in the design problem, as the optimality criteria depends on these unknown parameters (Atkinson et al., 2007; Burkner et al., 2019). To address this challenge, researchers proposed various solutions, including local optimal designs (Aminnejad & Jafari, 2017; Chernoff, 1953; Dette et al., 2013; Ford et al., 1992), sequential optimal designs, minimax optimal designs, Bayesian optimal designs (Pilz, 1991; Parsamaram & Jafari, 2015; Goudarzi et al., 2019; Grashoff et al., 2012; Kiefer, 1959; Kiefer & Wolfowitz, 1959; Kiefer, 1974), and pseudo-Bayesian designs (Kiefer & Wolfowitz, 1959). Chernoff (1953) proposed to use a suitable guess of the parameter value which leads to locally optimal design. This approach aimed to overcome the difficulties associated with the dependence of the design problem on unknown parameters in nonlinear models. It's important to note that local designs for nonlinear models are derived subsequent to an initial linearization of the model, using the parameter set as a reference point.

The selection of unknown parameters in local designs is typically obtained from previous studies or experiments specifically conducted for this purpose. The sensitivity of the locally optimal design with respect to the initial guess of parameter value is demonstrated by Dette et al. (2013); Rodriguez-Torreblanca and Rodríguez-Díaz, (2007). A locally optimal design do not incorporate any uncertainty in the parameter values. One of the proposed approaches, which deals with the uncertainty in parameter values, is the Bayesian procedure that assumes a prior distribution for the parameter. In the Bayesian method, the first step is to represent the available information in the form of a probability distribution for the model parameter, known as the prior distribution. So that, the idea of the Bayesian optimal design is to use the informative and/or historical knowledge of the unknown parameters as prior distribution. A Bayesian optimal design aims to maximize the relevant optimality criterion over this prior distribution. Nevertheless, it is crucial to acknowledge that the selection of the prior distribution within the Bayesian framework can be problematic and may potentially lead to erroneous results. The choice of the prior distribution is subjective, relying on the researcher's beliefs, and it significantly influences the final outcome. Unfortunately, the Bayesian approach lacks a definitive method for selecting the prior distribution. Subjective specification of a prior distribution which captures all existing information about the uncertainty of the parameter values was employed by many authors such as Chaloner and Larentz (1989); Chaloner and Duncan (1983); Burghaus and Dette (2014); Chaloner and Vardinelli (1995); Pronzato and Walter (1985); Mukhopadhyay and Haines (1995); Dette and Ngobauer (1996); Dette and Ngobauer (1997); Fedorov and Hackl (2012); Fedorov and Leonov, (2013); Firth and Hinde (1997) that have contributed extensively to this field. Chapter 18 of Atkinson et al. (2007) book provides further reading on this topic. Often the choice of the prior is a compromise of a representation of uncertainty of the parameter values that may not be correct and can lead to misleading decision. Moreover, using the custom priors is a restrictive choice of priors, and it is possible to distort the actual prior distribution of the parameter. Indeed, no single probability distribution can model ignorance satisfactory, therefore large classes of distributions are needed. In this regards, we show that such a class is attained by considering infinite dimensional families of prior distributions; we consider the prior distribution function as an unknown distribution, which belongs to a class of distribution functions. Thus, from a Bayesian point of view, we need to construct a prior distribution on the space of all distribution functions. Several methods were introduced to construct a prior for random distribution. In this paper, we apply a nonparametric Bayesian approach that puts a prior on such families. In nonparametric Bayesian analysis, the prior process in terms of a probability measure P instead of the corresponding distribution function is discussed. The Dirichlet process, which is defined by Ferguson (1973), plays a central role in nonparametric Bayesian methods. Dirichlet Process (DP) involved two desirable properties of a prior; First, DP is defined on an arbitrary probability space. Second, it belonged to a conjugate family of priors. The aim of this paper is to apply Dirichlet process priors to obtain the Bayesian D-optimal design.

This research paper presents the optimal design for nonlinear models in section 2. In Section3, the nonparametric Bayesian D-optimal design for exponential regresion model is presented. Finally, Section 4 concludes the paper with some closing remarks.

Introduction to Optimal Designs in Nonlinear Models

In the realm of nonlinear experimental design, a common scenario arises where in the relationship between the response variable y and the independent variable x is given by the equation $y = \eta(x, \theta)+\epsilon$ where x $\chi \subseteq$ R and y is a response variable and $\theta \in \Theta$ is the unknown parameter vector and ϵ is a normally distributed residual value with mean 0 and known variance $\sigma2 > 0$. For simplicity, we assume $\sigma2 = 1$ in this problem. If $\eta(x, \theta)$ is differentiable with respect to θ then, the information matrix M (ξ, θ) at a given point x can be represented as follows: Equation 1

$$I(\xi, \boldsymbol{\theta}) = \frac{\partial}{\partial \boldsymbol{\theta}} \eta(x, \boldsymbol{\theta}) \frac{\partial}{\partial \boldsymbol{\theta}^T} \eta(x, \boldsymbol{\theta}). \quad (1)$$

There exist several optimality criteria used to obtain the optimal design, including D-optimality and A-optimality. These criteria are functions of the information matrix and can be expressed as follows:

$$\Psi_D(\xi, \boldsymbol{\theta}) = -\log(\det(M(\xi, \boldsymbol{\theta}))) , \Psi_A(\xi, \boldsymbol{\theta}) = tr(M^{-1}(\xi; \boldsymbol{\theta}) \quad (2)$$

Where ξ denotes a design with two components; the first component represents specific values from the design space χ and the second component corresponds to the weights assigned to these values, so that design ξ can be defined as follows:

$$\xi = \begin{Bmatrix} x_1 & x_2 & \ldots & x_\ell \\ w_1 & w_2 & \ldots & w_\ell \end{Bmatrix} \in \Xi, \quad (3)$$

where p represents the number of model parameters (Kiefer, 1974), and

$$\Xi = \{\xi \mid 0 \le w_j \le 1 ; \sum_{j=1}^{\ell} w_j = 1 , x \in \boldsymbol{\chi}\}, p \le \ell \le \frac{p(p+1)}{2} \quad (4)$$

When considering a discrete probability measure ξ with finite support, the information function of ξ can be expressed as follows (Atkinson et al., 2007):

$$M(\xi, \boldsymbol{\theta}) = \sum_{j=1}^{\ell} w_j I(x_j, \boldsymbol{\theta}). \quad (5)$$

Because of the dependence of the information matrix M (ξ, θ) to the unknown parameter θ, one approach to address this issue is to employ the Bayesian method and incorporate a prior distribution of the parameter vector. The Bayesian D-optimality criterion can be formulated as follows:

$$\Psi_\Pi(\xi) = E(\psi(\xi; \boldsymbol{\theta})) = \int_\Theta \psi(\xi; \boldsymbol{\theta}) d\Pi(\boldsymbol{\theta}) = \int_\Theta -\log(\det(M(\xi, \boldsymbol{\theta}))) d\Pi(\boldsymbol{\theta}), \quad (6)$$

where Π represents the prior distribution for θ and the Bayesian D-optimal design is attained by minimizing (6).

In certain situations, specifying a prior distribution on the parameter space Θ can be challenging for the experimenter. In such cases, an alternative approach is to consider an unknown prior distribution Π for the parameter θ. In this condition, Π is treated as a parameter itself. Consequently, equation (6) becomes a random functional, and it becomes necessary to determine its distribution or approximation. From a Bayesian perspective, we construct a prior distribution on the space of all distribution functions to address this issue. To achieve this objective, Ferguson (1973) introduced the concept of the DP that an overview of it will be provided in the following.

Nonparametric Bayesian D-optimal design

Nonparametric models constitute an approach to model selection and fitting, where the size of the models is allowed to grow with the size of the data. It is unlike parametric models that use a fixed number of parameters. In this section, we introduce the nonparametric Bayesian optimal design. In the nonparametric Bayesian framework, it is assumed that $\theta \mid P \sim P$, where P is a random probability distribution and $P \sim \Pi$. General method of construction a random measure is to start with the stochastic processes. Ferguson (1973) formulated the requirements which must be imposed on a prior distribution and proposed a class of prior distributions, named DP (Teh, 2010). One of the main argument in using the Dirichlet distribution in practical applications is based on the fact that this distribution is a good approximation of many parametric probability distributions. Bondesson (1982); Sethuraman (1994); Zarepour and Al Labadi (2012) are among those who have contributed to this area. A method of producing samples from the Dirichlet process is to use the Polya urn process that in the upcoming section, we will discuss about it. Then the nonparametric Bayesian D-optimal design for the Exponential regresion model is discussed.

Polya Urn Scheme

Polya Urn Scheme was used by Blackwell and McQueen (1973) to demonstrate the existence of the Dirichlet Process. The method of producing a sample of the Dirichlet Process is to use a Polya Urn Scheme (Ghalanos & Theussl, (2015). Consider a Polya urn with a(χ) balls of which a(i) are of color i ; i = 1, 2, ..., k. [For the moment assume that a(i) are whole numbers or 0]. Draw balls at random from the urn, replacing each ball drawn by two balls of the same color. *Let* $X_i = j$ if the i th ball is of color j. Then:

$$P(X_1 = j) = \frac{a(j)}{a(\chi)}, \tag{7}$$

$$P(X_2 = j \mid X_1) = \frac{a(j) + \delta_{X_1}(j)}{a(\chi) + 1}, \tag{8}$$

and in general

$$P(X_{n+1} = j \mid X_1, X_2, \ldots, X_n) = \frac{a(j) + \sum_1^n \delta_{X_i}(j)}{a(\chi) + n}, \tag{9}$$

That n is the number of extracted balls and $\delta_X(j)$ is equal to one if $X_i = j$, otherwise it is equal to zero.

Nonparametric Bayesian D-optimal design for Exponential regresion model with Respect to Prior Processes (with Polya Urn Scheme as the base measure)

Suppose we have the following regression model:

$$E(y|x) = \eta(x, \boldsymbol{\theta}) = \exp(-\vartheta x),\ x > 0,\ \vartheta > 0. \tag{10}$$

therefore, the Bayesian D-optimality criterion, denoted as ΨΠ(ξ) can be expressed as follows:

$$\Psi_\Pi(\xi) = E(\psi(\xi; \boldsymbol{\theta})) = \int_\Theta \psi(\xi; \vartheta)\, d\Pi(\boldsymbol{\theta}) = \int_\Theta -\log \sum_{j=1} w_j x_j^2[\exp(-2\vartheta x_j)])\, d\Pi(\vartheta) \tag{11}$$

where Π is the prior distribution for θ. The Bayesian D-optimal design is attained by minimizing equation (11). In the nonparametric Bayesian framework, we consider $P \sim \mathrm{DP}(\alpha, P_0)$ and its collective representation as $P(.) = \sum_{i=1}^{\infty} p_i\, \delta_{\vartheta_i}(.)$. In this context, the optimality criterion can be expressed as follows:

$$\Psi_\Pi(\xi) = \sum_{i=1}^{\infty} p_i(-\log \sum_{j=1}^{k} w_j x_j^2[\exp(-2\vartheta_i x_j)]). \tag{12}$$

Chernoff (1953) demonstrated that when searching for a local optimal design, there exists an optimal design where all the mass is concentrated at a single point within the design supports. Caratheodory's theorem also confirms the existence of a one-point optimal design. However, when employing the Bayesian optimality criterion, a more complex situation arises. Dette and Neugebauer, (1996) showed that with a uniform prior distribution, as the support of the prior distribution increases, the number of optimal design points for the single-parameter model also increases. Chaloner and Verdinelli (1995) suggested that if the researcher aims to obtain a one-point optimal design, it is advisable to consider a small support for the uniform prior distribution. The same principle applies to nonparametric Bayesian designs. In this case, assuming a uniform distribution over the interval [0, B] as the basic distribution, the one-point optimal design can be achieved.

Equation (11) is a stochastic function of the DP. According to Ferguson's definition of the DP, the calculation (3.2) is not easily possible, so to address this challenge and obtain an approximation of the optimal nonparametric Bayesian criterion, methods such as the stick-breaking process is employed. Sethuraman (1994) introduced this method as a significant approach for generating realizations of the DP. Another method has been presented by Zarepour and Ellabadi (2012) whose simulation speed and accuracy is much higher than the stick breaking process. We used this method in this paper.

Now, in this section we consider Polya Urn Scheme as the base measure in DP. We get the results by using a nonlinear optimization programing with R package Rsolnp (Ghalanos & Theussl, 2015). To better understanding of the effect of the α parameter, we tabulate the results for four different values of α=1, 5, 10, 50, in Tables 1-4. Without loss of generality, we consider a bounded design space χ=[0, 1]. Tables 1-4 represent the results when the concentration parameter and uncertainty in the base measure increase. According to the results, when the value of α increases, the support points in two points design do not significantly change. The weight of minimum point increases rapidly and the smallest point will have the most weight that this weight almost increases or remains fixed by increasing the concentration parameter. Also for three points design, minimum support point has the greatest weight. In addition, in the range under investigation, the results show that we do not have a three point design for μ = 5, σ = 2, and in fact, it converts to the design by less points. This observation is more clear for larger concentration parameter. But, by increasing the parameter space, optimal two and three point designs are obtained.

Table 1: Nonparametric Bayesian D-optimal designs with truncated normal base distribution and concentration parameter when α=1

Parameters	Design	Two points	Three points
μ = 5, σ = 2	x	0.223238 0.672626	– – –
	w	0.971536 0.028464	– – –
μ = 50, σ = 30	x	0.020751 0.189805	0.018863 0.193065 0.299221
	w	0.959810 0.040190	0.993434 0.003970 0.002596
μ = 150, σ = 90	x	0.007980 0.197085	0.007751 0.193707 0.299374
	w	0.980722 0.019278	0.988099 0.010318 0.001583
μ = 1000, σ = 500	x	0.001488 0.198136	0.001354 0.200019 0.299828
	w	0.998521 0.001479	0.999742 0.000128 0.000130

Table 2: Nonparametric Bayesian D-optimal designs with truncated normal base distribution and concentration parameter when α=5.

Parameters	Design	Two points	Three points
μ = 5, σ = 2	x	0.323630 0.581538	– – –
	w	0.555981 0.444019	– – –
μ = 50, σ = 30	x	0.018351 0.189065	0.018444 0.183531 0.299077
	w	0.942754 0.057246	0.986648 0.007353 0.005999
μ = 150, σ = 90	x	0.006745 0.187195	0.006462 0.188178 0.298479
	w	0.973256 0.026744	0.986702 0.012083 0.001215
μ = 1000, σ = 500	x	0.001035 0.195904	0.001048 0.198217 0.300620
	w	0.996235 0.003765	0.999070 0.000768 0.000162

Now, if we assume the mean of the base distribution to be constant and increase the variance, it can be seen that in the two point designs, the smallest point has the most weight. The results related to this case has been presented in the table 5.

Table 3: Nonparametric Bayesian D-optimal designs with truncated normal base distribution and concentration parameter when α=10.

Parameters	Design	Two points	Three points
μ = 5, σ = 2	x	0.207276 0.599491	– – –
	w	0.769156 0.230844	– – –
μ = 50, σ = 30	x	0.017722 0.201868	0.018066 0.182005 0.302160
	w	0.945074 0.054926	0.990114 0.002937 0.006949
μ = 150, σ = 90	x	0.006342 0.181494	0.006414 0.179023 0.295396
	w	0.971519 0.028481	0.988448 0.010337 0.001215
μ = 1000, σ = 500	x	0.000999 0.195064	0.000992 0.197084 0.300800
	w	0.996286 0.003714	0.998194 0.001709 0.000097

Table 4: Nonparametric Bayesian D-optimal designs with truncated normal base distribution and concentration parameter when α=50.

Parameters	Design	Two points	Three points
μ = 5, σ = 2	*x*	0.196904 0.299491	– – –
	w	0.769156 0.230844	– – –
μ = 50, σ = 30	*x*	0.018481 0.230227	0.018248 0.177483 0.311380
	w	0.972158 0.027842	0.989506 0.002450 0.008044
μ = 150, σ = 90	*x*	0.006263 0.176120	0.006218 0.171950 0.301432
	w	0.979629 0.020371	0.992705 0.004860 0.002435
μ = 1000, σ = 500	*x*	0.000971 0.193872	0.000984 0.193383 0.300319
	w	0.995262 0.004738	0.997486 0.002201 0.000313

Table 5: Nonparametric Bayesian D-optimal designs with truncated normal base distribution and concentration parameter when α=1

Parameters	Design	Two points	Three points
μ = 5,0 σ = 30	*x*	0.022991 0.191695	0.019425 0.191129 0.296905
	w	0.945594 0.054406	0.992596 0.006730 0.000674
μ = 50, σ = 90	*x*	0.014683 0.196830	0.013089 0.187962 0.302637
	w	0.936699 0.01281	0.063304 0.023552 0.000484
μ = 50, σ = 500	*x*	0.004969 0.192861	0.004082 0.191850 0.300626
	w	0.968402 0.031598	0.989670 0.010321 0.000007

Concluding Remarks and Future Works

Nonlinear regression models are widely used in various scientific fields, and the Bayesian method is commonly employed to obtain optimal designs in such models. However, one of the challenges in the Bayesian framework is the subjective selection of the prior distribution, which can potentially lead to incorrect results. The choice of the prior distribution is often based on the researcher's beliefs, and it strongly influences the final outcome. Unfortunately, the Bayesian approach lacks a systematic method for selecting the prior distribution. To overcome these limitations and reduce reliance on restrictive parametric assumptions, nonparametric Bayesian methods are pursued. In this study, we consider the prior distribution as an unknown parameter and utilize the Dirichlet process to derive nonparametric Bayesian D-optimal designs. Specifically, we focus on a nonlinear model with one parameter, namely the Unit-Exponential distribution. We investigate the Bayesian D-optimal design for the exponential regression model using a truncated normal prior distribution, examining various parameter values. By adopting a nonparametric Bayesian approach and utilizing the Dirichlet Process, we aim to address the challenges associated with selecting the prior distribution in Bayesian optimal design construction. This allows us to account for uncertainty and mitigate the impact of restrictive parametric assumptions, providing more flexible and robust designs for nonlinear regression models.

In this study, we focus on utilizing the Polya Urn Scheme as the base distribution in the Dirichlet Process. To better understand the influence of the concentration parameter α, we present the results in tables for four different values of α=1, 5, 10, 50. These tables provide valuable insights into the nonparametric Bayesian optimal designs, showcasing the distribution of weights and support points. By analyzing the results for different values of α, we can better understand the impact of this parameter on the design outcomes. This approach allows us to explore and evaluate the performance of the nonparametric Bayesian optimal designs under varying levels of concentration parameter α.

In the investigated range, the results reveal interesting findings. For small parameter values, there are no three-point designs observed. However, By increasing uncertainty in the base measure, another optimal point is obtained with a very small weight, resulting in a design where the smallest point has the highest weight.

Moreover, as the uncertainty in the base measure and the concentration parameter in the Dirichlet Process increase, the support points in the two-point designs do not undergo significant changes. The weight of the smallest point increases rapidly, and it becomes the point with the highest weight. This weight tends to either increase or remain relatively stable with an increase in the concentration parameter.

It is important to note that this approach can be applied to other optimality criteria and various models with two or more parameters. For example, nonparametric Bayesian optimal designs using the A- or E-optimality criterion for the nonlinear model discussed in this paper, along with a Dirichlet process prior, hold potential for further research. We hope to report new results in this area in the near future.

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