Bayesian Optimal Experimental Design for Generalized Linear Models.

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Abstract

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1. Introduction

One of the main challenges in scientific research is the design of an experiment. A good experimental design will make the difference between finding an answer to our research question and wasting valuable resources. Optimal Experimental Design (OED) allows us to re-interpret the design of an experiment as a decision problem where the objective is to maximize a utility function. This function is a representation of our preferences over the possible results of the experiment.

To optimize the design of an experiment, first we need to identify which of our variables are subject to this procedure. For example, we might want to select which values of an independent variable should be tested, or how many times we should test each of those values. Most of the time, these choices are made on the basis of previous research. However, it might be the case that there is not enough information to make these decisions with confidence, or that the values that are commonly used, do not allow for strong conclusions. Second, we need to formalize the objective of the experiment through a utility function. There are two examples in the literature that use different functions (Myung and Pitt, 2009; Zhang and Lee, 2010, e.g.), in both examples the objective is to discriminate between competing cognitive models. Nonetheless, considerations of what makes a model "good" drive the authors to choose different functions.

In this paper, we will present a different approach where the problem is not to select between models but to make inferences about the parameters of a single one. In particular, we will present an example of OED with a model that is commonly used in Psychophysics and Decision Making, the logistic response model. In this example, we will optimize an experimental design focused on studying the ability of participants to detect changes in the success rate of a probabilistic series. Additionally, we will show how different prior assumptions can change the results obtained from this process, this will highlight the importance of the choice of prior distributions in the process of designing an experiment. It is important to note that the aproach presented here follows a Bayesian perspective of optimal designs for GLM. A good introduction to othe approaches and their limitations can be found in Khuri et al. (2006).

The rest of the paper will be organized in the following way. First, we will introduce the concepts of OED particularly in the field of Generalized linear models. Second, we will present a brief summary of the experimental problem being addressed and, a computational model which has been used to account for the behavior of human participants under similar settings. Finally, we will present the results of the optimization procedure under different prior distributions, including one generated from the model responses to simulations of the experiment.

2. Optimal experimental design

To apply the concepts of OED to a particular problem, first, we need to define the elements of the design space. This space is conformed by the variables that we can manipulate during the experiment, for example, the values that our independent variable might take or the weight (proportion of observations) assigned to each of those values. These elements are the ones that we can modify in order to optimize the design.

The second step would be to formalise the objective of the experiment. For example, in the case of a logistic model, we might want to find the values of our independent variable that minimize the variance of the model parameters, or we might be interested in the magnitude of the physical stimulus for which the probability of a response takes on a certain value. The formalization of the research question will define a utility function.

The last step is to specify the prior information that we have about the problem at hand. This last step can be carried out in two ways, first, we can try to optimize the experiment for a particular guess about the parameter values of the model of interest, or we could use a probability distribution to account for the uncertainty in the values that we are interested in. This last step is primarily important to the optimization process in generalized linear models, because the optimal design will depend on the values of the parameters.

Once we have defined the design space η, the objective of the experiment and the prior informartion $p(\theta)$, the expected utility of a design is represented by the following equation:

$$U(\eta) = \int \int U(\eta, y, \theta) p(\theta|y, \eta) p(y|\eta) d\theta dy \tag{1}$$

Therefore, finding the experimental design that is optimal given a utility function, reduces to the problem of finding the values for the variables in η for which equation 1 takes it's maximum value.

Many utility functions have been proposed for both linear and non-linear design problems, however, as was previously mentioned, the choice of a utility function depends on the research question. For example, Myung and Pitt (2009) utilizes the sum of squered errors between the data generated by a model and the predictions of a competing one given an expeirmental design. This is because, the objective is to find a design that can discriminate the predictions of the two. On the other hand, Zhang and Lee (2010) choose a utility function based on the Bayes Factor. Both of this functions will have their advantages, nontheless, the first utility emphasizes disciminability of model's predictions, while the second one aims for a design in which the data generating model is more likely.

When the objective of the experiment is to make an inference about the parameters of a generalized linear model, some authors (e.g. Bernardo, 1979) have proposed to consider the gain in Shanon's Information as a utility function. In this case, the objective is to find the design η that maximizes the expected gain in Shanon Information, or equivalently, maximizes the Kullback-Leibler divergence between the posterior and prior distribution. With this function, the expected utility of an experimental design is represented by the following equation:

$$U(\eta) = \int\int log\frac{p(\theta|y,\eta)}{p(\theta)}p(y,\theta|\eta)d\theta dy \tag{2}$$

The prior distribution in the denominator of the logarithm can be droped as it does not depend on the experimental design, therefore, the optimal design will be the one that maximizes:

$$U(\eta) = \int\int log\{p(\theta|y,\eta)\}p(y,\theta|\eta)d\theta dy \tag{3}$$

Which is the posterior expected Shanon information.

When dealing with generalized linear models, the posterior distribution of the parameter vector θ is not always tractable, however, in the literature of design optimization it is common to use the following aproximation to the posterior distribution

$$\theta|y,\eta \sim N\left(\hat{\theta}, [nI(\hat{\theta},\eta)]^{-1}\right) \tag{4}$$

Where $I(\hat{\theta},\eta)$ denotes the observed fisher information matrix given an experimental design and $\hat{\theta}$ is the maximum likelihood estimate of θ. Even with this, the marginal distribution of the data ($p(y|\eta)$) in equation 1 also needs to be aproximated, however, when the posterior utility only depends on y through some constistent estimate of $\hat{\theta}$, a further approximation is to take the predictive distribution of $\hat{\theta}$ to be the prior distribution Chaloner and Larntz (1989).

With both aproximations, the value of $U(\eta)$ is:

$$U(\eta) = -\frac{k}{2}log(2\pi) - \frac{k}{2} + \frac{1}{2}\int log\{det[nI(\theta,\eta)]\}p(\theta)d\theta \tag{5}$$

Equation 5 gives the exact expected utility of an esperimental design. However, one could drop the constant and multiplier terms giving the following form:

$$\phi(\eta) = \int log\{det[nI(\theta, \eta)]\}p(\theta)d\theta \tag{6}$$

The function $\phi(\eta)$ is known as a design critirion. An optimal design would be the one maximizing equation 6, nontheless, it is worth noting that this relies on the normal approximation to the posterior distribution in 4, therefore, for small smaples there are some constraints that help to assure normality (see Clyde and Chaloner, 2002).

3. OUTLINE

4. Optimal Experimental Design: Example

Why is is detecting changes important for an organism?

Change detection in probabilistic series.

Arising problems with experimental design.

Research question and its statistichal interpretation

Assumtion about the relationship between a subjects response the dependent variable under study

Design space for this problem and how to reduce the dimensionality of the space by assuming experimental constraints.

Utility function and its relationship with the objective of the experiment

Arising problems with utility function and the proposed response function. Bayesian solution, assigning a prior distribution to the parameters, the less research in a field the more difficult it is to assign an informative prior, however, we could use other cognitive models in order to propose a prior distribution.

4.1. Using a model to generate prior distributions

Using the prior distribution, the utility function and the definition of a design space we can otimize the experimental design in this case we are looking for $\delta\theta^*$ that maximizes the following equation:

$$U(\delta\theta^*) = \max_{\delta\theta} \int_{\beta} log(det(I(\beta|\delta\theta)))\pi(\beta)d\beta \tag{7}$$

The previous integral can be approximated via Monte Carlo sampling

5. Results

5.1. Consruction of the prior distribution

Prior over model parameters(Gallistel et al 2014) Results Constructing the prior: we take a multivariate normal distribution with mean and covariance equal to the unbiased estimators for both parameters.

5.2. Optimal design

Aproximating the utility function (integral) throught Monte Carlo simulation Utility aproximation for 2 Design points

the approximation returns a smooth curve over the 2 point design space.

6. Discussion

Optimal design for the example Properties of the most useful points (they land on the points of the curve where the steepness changes most dramatically)

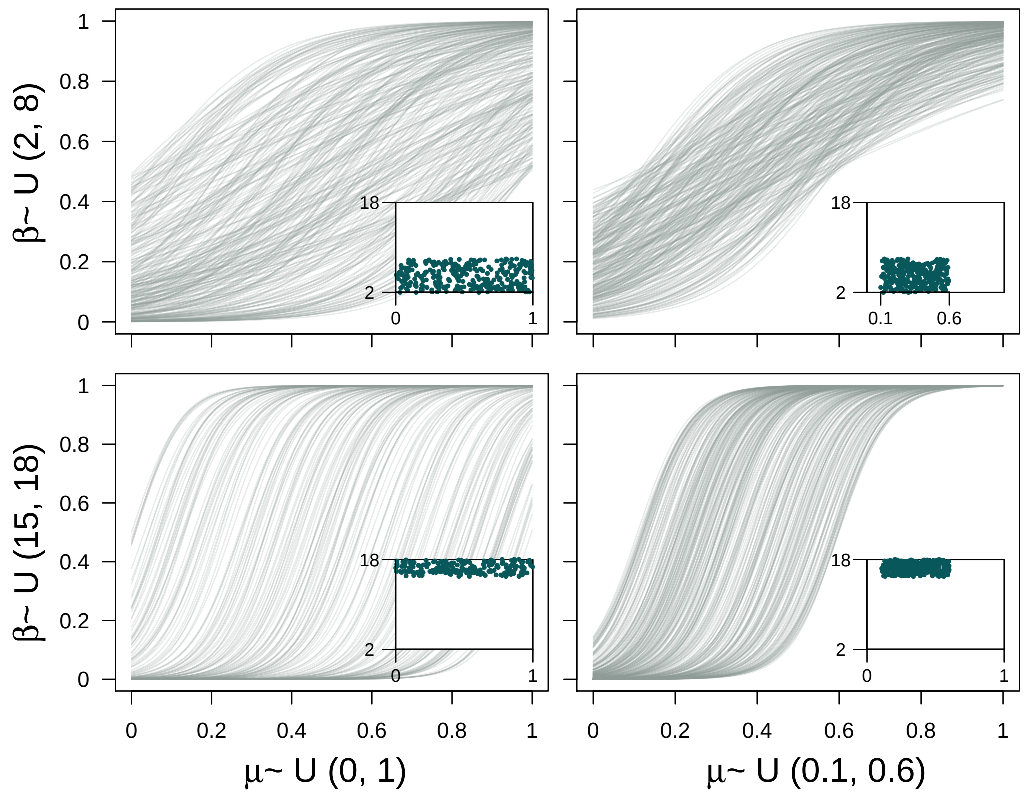

Figure 1: Prior and predictive prior distributions.

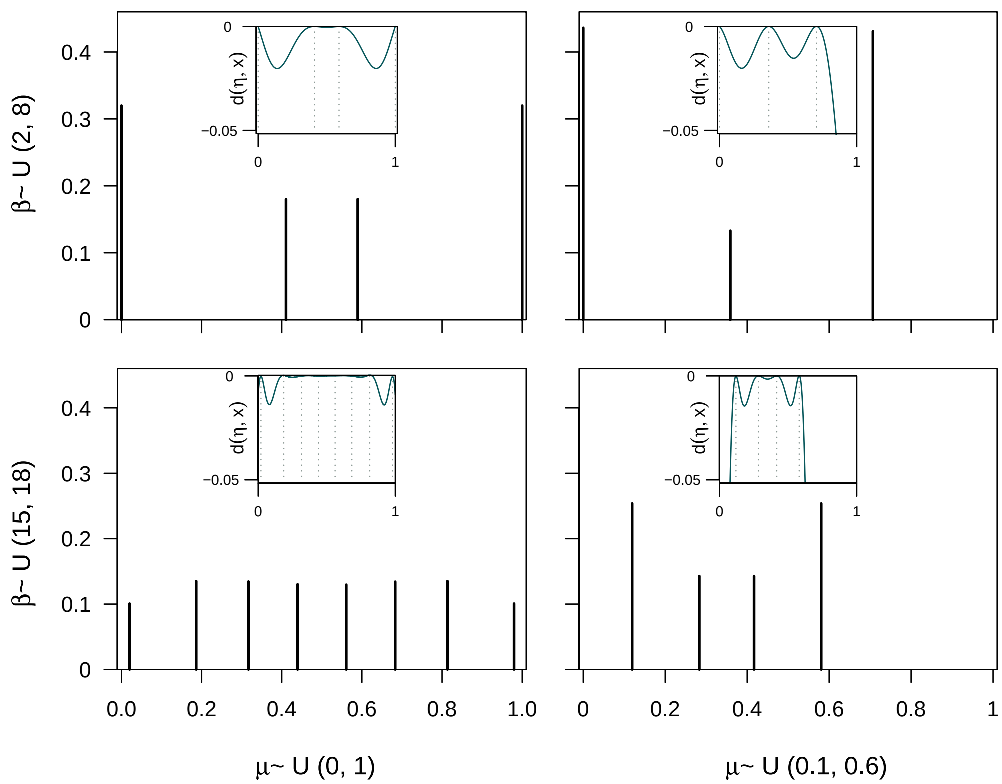

Figure 2: Optimal experimental designs and directional derivatives.

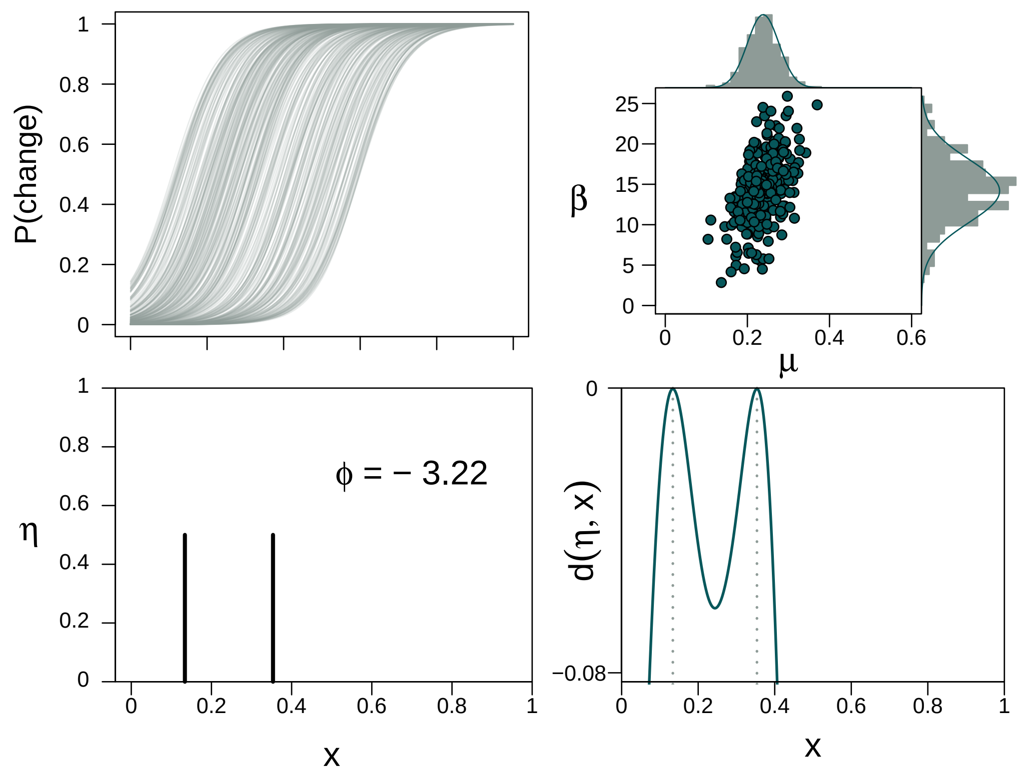

Figure 3: Informative prior distribution, prior predictive, optimal design and directional derivative.

Advantages of Optimal Design

Using models to generte prior distributions.

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