

# Geometry of Parameter Regions for Optimal Designs

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## 1 Introduction

Optimal design theory for nonlinear regression studies local optimality on a given design space. We identify the Bradley-Terry paired comparison model with graph representations and prove for an arbitrary number of parameters, that every saturated D-optimal design is displayed as a path in the graph representation. Via this path property we give a complete description of the optimality regions of saturated designs. Furthermore, we exemplify the unsaturated D-optimal designs with full support for 4 parameters.

## 2 Formulation of the problem

We consider pairs  $(i, j)$  of alternatives  $i, j = 1, \dots, n$ . The preference for  $i$  over  $j$  is denoted in a binary variable  $Y(i, j)$  with  $Y(i, j) = 1$ , if  $i$  is preferred over  $j$  and  $Y(i, j) = 0$  otherwise. We assume, that there is a ranking for the alternatives via some constants  $\pi_i$ , so that the preference probability is

$$\mathbb{P}(Y(i, j) = 1) = \frac{\pi_i}{\pi_i + \pi_j}.$$

The model is transformed into a logistic model with  $\beta_i := \log(\pi_i)$ :

$$\mathbb{P}(Y(i, j) = 1) = \frac{1}{1 + \exp(-(\beta_i - \beta_j))} = \eta(\beta_i - \beta_j)$$

with  $\eta(z) = (1 + \exp(-z))^{-1}$  as the inverse logit link function. As the preference probabilities only depend on the relation of the  $\pi_i$ , we are allowed to set  $\pi_n = 1$  and therefore  $\beta_n = 0$ . The possibility to fix one of the parameters is known in general as the identifiability condition, the case with  $\beta_n = 0$  as control coding. W.l.o.g. assume  $i < j$ . Furthermore,  $e_i$  is the  $(n - 1)$ -dimensional unit vector. Then, we choose

$$f(i, j) = \begin{cases} e_i - e_j, & \text{for } i, j \neq n \\ e_i, & \text{for } (i, n) \end{cases}$$

as the regression vector, so that

$$\mathbb{P}(Y(i, j) = 1) = \eta(f(i, j)^\top \beta)$$

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with  $\beta^\top = (\beta_1, \dots, \beta_{n-1})$ . Then, the Information matrix of a design point  $(i, j)$  is

$$M((i, j), \beta) = \lambda_{ij} f(i, j) f(i, j)^\top$$

with the intensity  $\lambda_{ij} := \lambda_{i,j}(\beta) = \frac{e^{\beta_i - \beta_j}}{(1 + e^{\beta_i - \beta_j})^2}$ . The Information matrix of the model for a design  $\xi$  with weights  $w_{ij}$  is then given by

$$M(\xi, \beta) = \sum_{(i,j)} w_{ij} M((i, j), \beta) = \sum_{(i,j)} w_{ij} \lambda_{ij} f(i, j) f(i, j)^\top.$$

The celebrated equivalence theorem (compare for example [1]) states that a design  $\xi^*$  is locally D-optimal if and only if

$$\lambda_{ij} f(i, j)^\top M(\xi^*, \beta)^{-1} f(i, j) \leq n - 1$$

for all  $1 \leq i < j \leq n$ . So, the optimality regions of a design is given as a semialgebraic set, hence a set of polynomial equations and inequalities in the weights and the intensities. This enables us to apply tools from computer algebra to study the optimality regions of both saturated and unsaturated designs and to extend the results from [2] to 4 alternatives. Furthermore, we connect saturated designs with graph representations and proof the following theorem:

**Theorem 2.1** *In the Bradley-Terry paired comparison model, every saturated optimal designs graph representation is a path, so a graph in which every node has at most two neighbours.*

## References

- [1] Silvey S.D. *Optimal design: an introduction to the theory for parameter estimation* // Chapman and Hall, 1980.
- [2] Graßhoff U., Schwabe R. *Optimal design for the Bradley-Terry paired comparison model* // Statistical Methods and Applications, 2008, v. 17, n. 3, p. 275-289.