# On the feasibility of semi-algebraic sets in Poisson regression

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**Abstract.** Designing experiments for generalized linear models is difficult because optimal designs depend on unknown parameters. The local optimality approach is to study the regions in parameter space where a given design is optimal. In many situations these regions are semi-algebraic. We investigate regions of optimality using computer tools such as YALMIP, QEPCAD, and MATHEMATICA.

**Keywords:** algebraic statistics, optimal experimental design, Poisson regression, semi-algebraic sets

## 1 Introduction

Generalized linear models are a mainstay of statistics, but optimal experimental designs for them are hard to find, as they depend on unknown parameters of the model. A common approach to this problem is to study local optimality, that is, determine an optimal design for each fixed set of parameters. In practice, this means that appropriate parameters have to be guessed a priori, or fixed by other means. In [12] the authors approached this problem from a global perspective. They study the regions of optimality of fixed designs and demonstrate that these are often defined by semi-algebraic constraints. Their main tool is a general equivalence theorem due to Kiefer and Wolfowitz, which directly yields polynomial inequalities in the parameters. This makes these problems amenable to the toolbox of real algebraic geometry. In this extended abstract we pursue this direction for the Rasch Poisson counts model which is used in psychometry [6] in the design of mental speed tests. Analyzing saturated designs for this model amounts to studying the feasibility of polynomial inequality systems. We examine the state of computer algebra tools for this purpose and find that there is room for improvement.

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## 2 Polynomial inequality systems in statistics

For brevity we omit any details of statistical theory and focus on mathematical and computational problems. The interested reader should consult [12] and its references. We also stick to that paper's notation. Throughout, fix a positive integer k, the number of rules, and another positive integer  $d \le k$ , the interaction order. A rule setting is a binary string  $x = (x_1, \ldots, x_k) \in \{0, 1\}^k$ . The regression function of interaction order d is the function  $f: \{0, 1\}^k \to \{0, 1\}^p$  whose components are all square-free monomials of degree at most d in the indeterminates  $x_1, \ldots, x_k$ . The value p equals the number of square-free monomials of degree at most d and depends on d and k. For any  $\beta \in \mathbb{R}^p$ , the intensity of the rule setting  $x \in \{0, 1\}^k$  is

$$\lambda(x,\beta) = e^{f(x)^T \beta}.$$

The information matrix of x at  $\beta$  is the rank one matrix

$$M(x, \beta) = \lambda(\beta, x) f(x) f(x)^{T}$$
.

The information matrix polytope is

$$P(\beta) = \text{conv}\{M(x,\beta) : x \in \{0,1\}^k\}.$$

The case d = 1 and k arbitrary is known as the model with k independent rules. In this case  $f(x) = (1, x_1, ..., x_k)$  and p = 1 + k. Then P(0) is known as the correlation polytope, a well studied polytope in combinatorial optimization. This case is particularly well-behaved, well-studied, and relevant for practitioners. It was investigated in depth in [7,8,9,12].

The pairwise interaction model arises for d = 2, where

$$f(x) = (1, x_1, \dots, x_k, x_1 x_2, x_1 x_3, \dots, x_{k-1} x_k)$$

and  $p = 1 + k + {k \choose 2}$ . This situation is already so intricate that neither an algebraic description of the model (the set of vectors  $(\lambda(x,\beta))_{x\in\{0,1\}^k}$  parametrized by  $\beta\in\mathbb{R}^p$ ) nor an explicit description of the polytope  $P(\beta)$  are known.

An approximate design is a vector  $(w_x)_{x\in\{0,1\}^k} \in [0,1]^{2^k}$  of non-negative weights with  $\sum_x w_x = 1$ . To each approximate design there is a matrix  $M(w,\beta) = \sum_x w_x M(x,\beta) \in P(\beta)$ . The main problem of classical design theory is to find designs w that are optimal with regard to some criterion. We limit ourselves to D-optimality, where the determinant ought to be maximized. To simplify the problem, we also only consider maximizing the determinant over  $P(\beta)$ , and not finding explicit weights w that realize an optimal matrix in  $P(\beta)$ . In non-linear regression, such as the Poisson regression considered here, this optimal solution depends on  $\beta$  (in linear regression it does not). Our approach is to consider the set of optimization problems for all  $\beta$  and subdivide them into regions where the optima are structurally similar. These regions of optimality are semi-algebraic.

In our setting, there are always matrices with positive determinant in  $P(\beta)$ . Since the vertices are rank one matrices, the optimum cannot be attained on

any face that is the convex hull of fewer than p vertices. A design w is saturated if it achieves this lower bound, that is,  $|\operatorname{supp}(w)| = p$ .

As the logarithm of the determinant is concave, for each given  $\beta$ , the optimization problem can be treated with the tools of convex optimization. The design problem is to determine the changes in the optimal solution as  $\beta$  varies.

A special design, relevant for practitioners and studied in [12], is the corner design  $w_{k,d}^*$ . It is the saturated design with equal weights  $w_x = 1/p$  for all  $x \in \{0,1\}^k$  with  $|x|_1 \le d$ . For example, for k=3 rules and interaction order d=2 the regression function is  $f(x_1,x_2,x_3)=(1,x_1,x_2,x_3,x_1x_2,x_1x_3,x_2x_3)$  and there are p=7 parameters. The corner design has weight 1/7 on the seven binary 3-vectors different from (1,1,1).

Saturated designs are mathematically attractive due to their combinatorial nature. It is reflected in the following classical theorem of Kiefer and Wolfowitz which is a main tool in the theory of optimal designs. See [15, Section 9.4] or [13] for details and proofs.

**Theorem 1.** Let  $X \subset \{0,1\}^k$  be of size p. There is a matrix with optimal determinant in the face  $\operatorname{conv}\{M(x,\beta): x \in X\}$  if and only if for all  $x \in \{0,1\}^k$ 

$$\lambda(x,\beta)(F^{-T}f(x))^T\psi^{-1}(\beta)(F^{-T}f(x)) \le 1.$$

where F is the  $(p \times p)$ -matrix with rows  $f(x), x \in X$  and  $\psi$  is the diagonal matrix  $\operatorname{diag}(e^{\beta_1}, \ldots, e^{\beta_p})$ . If this is the case, then the optimal point is  $\frac{1}{p} \sum_{x \in X} M(x, \beta)$ , the geometric center of the face.

After changing the scale by the introduction of parameters  $\mu_i = e^{\beta_i}$ , Theorem 1 yields a system of rational polynomial inequalities in the  $\mu_i$ . Together with the requirements  $\mu_i > 0$ , we find a semi-algebraic characterization of regions of optimality for saturated designs.

For example, the inequalities corresponding to the corner design are the topic of [12]. It can be seen that there always exist parameters  $\beta_1, \ldots, \beta_p$  that satisfy the inequalities in Theorem 1. A good benchmark for our understanding of the semi-algebraic geometry of the Rasch Poisson counts model is to understand the other saturated designs, raised as [12, Question 3.7].

Question 1. When  $\beta_i < 0$ , for all i = 1, ..., p, is the corner design the only saturated design w that admits parameters  $\beta$  such w is D-optimal for  $\beta$ ?

For d=1, k=3, Question 1 has been answered by Graßhoff et al. They have shown that, up to fractional factorial designs at  $\beta=0$ , only the corner design yields a feasible system [9]. Using computer algebra, the case d=1, k=4 can be attacked.

## 3 Non-optimality of saturated designs for four predictors

Our benchmark problem for computational treatment of inequality systems is an extension of the content of [9] to the case d = 1 and k = 4. Together with

looking among them is the following.

Philipp Meissner, at the time of writing a master student, we have undertaken computational experiments. In this situation p=5 and a saturated design is specified by a choice of its support  $X \subset \{0,1\}^4$  with |X|=5. A number of reductions applies. For example, if all 5 points lie in a three-dimensional cube, the determinant can be seen to be equal to zero throughout the face, so that optimality is precluded from the beginning. The hyperoctahedral symmetry acts on the designs and the inequalities. Therefore only one representative of each orbit has to be considered. After these reductions we are left with 17 systems of inequalities, one for each orbit of supports of saturated designs. One orbit corresponds to the corner design for which there always exist parameters at which it is optimal. It is conjectured that the remaining 16 saturated designs

admit no parameters under which they are optimal. Theorem 1 translates this conjecture into the infeasibility of 16 inequality systems. The most complicated

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\begin{split} 4\mu_1\mu_2\mu_3\mu_4 + \mu_1\mu_3 + \mu_1\mu_2 + 4\mu_2\mu_3 + \mu_4 - 9\mu_2\mu_3\mu_4 &\leq 0 \\ 4\mu_1\mu_2\mu_3\mu_4 + \mu_2\mu_3 + \mu_1\mu_2 + 4\mu_1\mu_3 + \mu_4 - 9\mu_1\mu_3\mu_4 &\leq 0 \\ 4\mu_1\mu_2\mu_3\mu_4 + \mu_2\mu_3 + \mu_1\mu_3 + 4\mu_1\mu_2 + \mu_4 - 9\mu_1\mu_2\mu_4 &\leq 0 \\ \mu_1\mu_2\mu_3\mu_4 + \mu_2\mu_3 + \mu_1\mu_3 + \mu_1\mu_2 + \mu_4 - 9\mu_1\mu_2\mu_3 &\leq 0 \\ \mu_1\mu_2\mu_3\mu_4 + \mu_1\mu_3 + \mu_2\mu_3 + 4\mu_1\mu_2 + 4\mu_4 - 9\mu_3\mu_4 &\leq 0 \\ \mu_1\mu_2\mu_3\mu_4 + \mu_1\mu_2 + 4\mu_1\mu_3 + \mu_2\mu_3 + 4\mu_4 - 9\mu_2\mu_4 &\leq 0 \\ \mu_1\mu_2\mu_3\mu_4 + \mu_1\mu_2 + 4\mu_2\mu_3 + \mu_1\mu_3 + 4\mu_4 - 9\mu_1\mu_4 &\leq 0 \\ \mu_1\mu_2\mu_3\mu_4 + 4\mu_1\mu_2 + 4\mu_2\mu_3 + \mu_1\mu_2 + \mu_4 - 9\mu_3 &\leq 0 \\ \mu_1\mu_2\mu_3\mu_4 + 4\mu_1\mu_2 + \mu_1\mu_3 + 4\mu_2\mu_3 + \mu_4 - 9\mu_2 &\leq 0 \\ \mu_1\mu_2\mu_3\mu_4 + 4\mu_1\mu_2 + \mu_1\mu_3 + 4\mu_2\mu_3 + \mu_4 - 9\mu_1 &\leq 0 \\ \mu_1\mu_2\mu_3\mu_4 + 4\mu_1\mu_2 + \mu_2\mu_3 + 4\mu_1\mu_3 + \mu_4 - 9\mu_1 &\leq 0 \\ 4\mu_1\mu_2\mu_3\mu_4 + \mu_1\mu_2 + \mu_1\mu_3 + \mu_2\mu_3 + 4\mu_4 - 9 &\leq 0 \\ \mu_1 &> 0, \quad \mu_2 &> 0, \quad \mu_3 &> 0, \quad \mu_4 &> 0. \end{split}
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The interested reader is invited to try her favorite method of showing infeasibility of this system. We have first tried SDP methods. In the best situation, they would yield an Positivstellensatz infeasibility certificate (maybe for a relaxation). For this we used YALMIP [14] together with the MOSEK solver [2] to set up moment relaxations. While in general this method works and is reasonably easy to set up, it is not applicable here as the infeasibility of the system seems to depend on the strictness of the inequalities  $\mu_i > 0$ . Since spectrahedra are closed, the SDP method only works with closed sets. Tricks like introducing a new variables which represents the inverses of the  $\mu_i$  lead to unbounded spectrahedra. Bounding these is equivalent to imposing an arbitrary bound  $\mu_i \geq \epsilon$ . With this the degrees of the Positivstellensatz certificate for infeasibility grow (quickly) when  $\epsilon \to 0$ . In total, the numerical method can give some intuition, but it is not feasible to yield proofs for the benchmark problem.

Our second attempt was to use QEPCAD [4], a somewhat dated open source implementation of quantifier elimination. The system is very easy to use, but unfortunately it seems to have problems already with small polynomial inequality

systems due to a faulty memory management in the underlying library SACLIB. There have been attempts to rectify the situation [17], but their source code is unavailable and the authors are unreachable.

Finally, we tried the closed source implementation of quantifier elimination in MATHEMATICA [16] and were positively surprised about its power. Its function REDUCE quickly yields that FALSE is equivalent to the existence of  $\mu_1, \ldots, \mu_4$  satisfying some of the 17 inequality systems. However, the benchmark system above seems out of reach. From here, the road is open to trying various semi-automatic tricks. For example, MATHEMATICA can confirm within a reasonable time frame that there is no solution to the above inequality system when  $\mu_3 = \mu_4$  is also imposed. A summary of our findings will appear in the forthcoming master thesis of Philipp Meissner.

### 4 Outlook

Whoever takes an experimental stance towards mathematics will, from time to time, be faced with polynomial systems of equations and inequalities. We have shown one such a situation coming from statistics here and there are more to be found from the various equivalence theorems in design theory [15].

Deciding if such a system has a solution is a basic task. The technology to solve it should be developed to a degree that a practitioner can just work with off the shelf software to study their polynomial systems. For systems of equations this is a reality. There are several active open source systems that abstract Gröbner bases computations to a degree that one can simply work with ideals [1,10,11]. For systems of polynomial inequalities, the situation is not so nice. The method to exactly decide feasibility of general polynomial inequality systems is quantifier elimination [3, Chapter 14]. The only viable open source software for quantifier elimination is QEPCAD which appears unmaintained for about a decade. There do exist closed implementations that seem to work much better, for example in MATHEMATICA. Whether one accepts a proof by computation in a closed source system is a contentious matter.

*Problem 1.* Develop a fast and user-friendly open source tool to study the feasibility of polynomial inequality systems with quantifier elimination.

We shall not fear the complexity theory. The documentation and use cases of QEPCAD demonstrate that many interesting applications were in the reach of quantifier elimination already a decade ago. Gröbner bases were deemed impractical in view of their complexity theory, yet they are an indispensable tool now. We hope that in the future exact methods in semi-algebraic geometry can be developed to the same extend as exact methods in algebraic geometry are developed.

Finally, for experimentation one can always resort to numerical methods. Via the Nullstellensatz and the various Positivstellensätze the optimization community has developed very efficient methods to deal with polynomial systems of equations and inequalities [5].

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