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Choice of second-order response surface designs for logistic and Poisson regression models

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Abstract: Response surface methodology is widely used for process development and optimisation, product design, and as part of the modern framework for robust parameter design. For normally distributed responses, the standard second-order designs such as the central composite design and the Box-Behnken design have relatively high *D* and *G* efficiencies. In situations where these designs are inappropriate, standard computer software can be used to construct *D*-optimal and *I*-optimal designs for fitting second-order models. When the response distribution is either binomial or Poisson, the choice of an appropriate design is not as straightforward. We illustrate the construction of *D*-optimal second-order designs for these situations and show that they are considerably better choices than the standard designs. We present an example applying this approach to optimisation of an etching process.

Keywords: Bayesian design; generalised linear models; optimal design; response surface methods.

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1 Introduction

Response surface methodology (RSM), introduced by Box and Wilson (1951), has become the standard framework for much of industrial experimentation, including process development and optimisation and product design and development. RSM is also the basis of the modern approach to robust parameter design (see Myers et al., 1992). For a recent review of RSM, see Myers et al. (2004). There are also three books devoted exclusively to various aspects of RSM; Khuri and Cornell (1996), Box and Draper (2007) and Myers et al. (2009).

Fitting a second-order model to the response variable(s) of interest is an integral aspect of RSM. Consequently, the development of appropriate second-order designs and guidance on how to use them is extremely important. There are many standard second-order RSM designs, including the central composite design (CCD) and its variations (the rotatable CCD, the spherical CCD, the small composite design, and the face-centred cube), the Box-Behnken design, the hybrid family of designs, and the Hoke designs. There are situations where standard designs are not always appropriate, such as unusual sample size requirements, non-standard blocking conditions and variations from the standard model. For these scenarios, optimal designs have been suggested and are used frequently in practice. Both *D*-optimal and *I*-optimal designs can be easily constructed using commercial software.

Another non-standard situation arises when the distribution of the response variable is non-normal. For example, the response may be a proportion such as a fraction non-conforming in which case the response distribution is binomial, or it may be a count such as the number of defects on a unit of product in which a logical choice for the response distribution is the Poisson. A widely-used approach to handing a non-normal response is to use a variance-stabilising transformation, such as a power family transformation, and to conduct the RSM model fitting and optimisation in the transformed metric. Another approach is to fit an appropriate generalised linear model to the response data. This is often a better approach than the use of transformations. For example, Myers et al. (2002) present an example where the response variable is a Poisson count and a square root transformation is employed. The resulting second-order model gives negative predictions of the transformed response in the region that is most likely to be of interest to the experimenters, clearly an impossible result. A generalised linear model with a Poisson response would be a better modelling approach because the predicted counts cannot be negative. Lewis et al. (2001) show that a generalised linear model is often preferable to a data transformation because it results in shorter confidence intervals on the mean response, a measure of model fit quality as well as potential prediction accuracy.

If the experimenter plans to fit a second-order model and has a response that is known to be non-normal but is a member of the exponential family (which includes the binomial, Poisson, exponential and gamma distributions), he or she must select an appropriate response surface design. One alternative is to use a standard design. Another alternative is to use an optimal design for the specific response distribution. Until recently, the construction of a *D*-optimal design for a generalised linear model was computationally prohibitive. We discuss this problem in the next section, construct several examples of *D*-optimal designs for the binomial and Poisson response distribution cases, and then compare the resulting designs with standard designs. The *D*-optimal designs are considerably better than the standard designs for both binomial and Poisson responses. We also present an example of using a *D*-optimal design for a Poisson response surface model applied to optimisation of an etching process.

2 Optimal designs for generalised linear models

A generalised linear model is an extension of ordinary normal-theory linear regression that encompasses both linear and non-linear models, and admits any response distribution that is a member of the exponential family. This includes the familiar normal distribution, as well as the binomial, negative binomial, Poisson, geometric, exponential, gamma and inverse normal distributions. A generalised linear model contains three elements:

1. a response distribution
2. a linear predictor that involves the design variables, say $\boldsymbol{x}'\boldsymbol{\beta}$
3. a link function g that relates the natural mean of the response distribution to the linear predictor, say $g(\mu) = \boldsymbol{x}'\boldsymbol{\beta}$.

See Myers and Montgomery (1997) for a tutorial on generalised linear models and Myers et al. (2002) for a more comprehensive presentation.

We are focusing on second-order response surface models, so the linear predictor will always be of the complete second-order model

$$\boldsymbol{x}'\boldsymbol{\beta} = \boldsymbol{\beta} + \sum_{i=1}^{k} \boldsymbol{\beta}_i \boldsymbol{x}_i + \sum_{i=1}^{k} \boldsymbol{\beta}_{ii} \boldsymbol{x}_i^2 + \sum_{i} \sum_{<j=2}^{k} \boldsymbol{\beta}_{ij} \boldsymbol{x}_i \boldsymbol{x}_j \tag{1}$$

where k is the number of design variables. The number of parameters in this model is $p = 1 + 2k + \frac{k(k-1)}{2}$. For the binomial response distribution, we will use the logistic link, so that the model the experimenter fits is

$$E(y) = \frac{e^{\boldsymbol{x}'\boldsymbol{\beta}}}{1 + e^{\boldsymbol{x}'\boldsymbol{\beta}}} \tag{2}$$

the familiar logistic regression model. For the Poisson response distribution, we will use the log link, resulting in the model

$$E(y) = e^{\boldsymbol{x}'\boldsymbol{\beta}} \tag{3}$$

Now consider finding *D*-optimal designs for these models. For the case of a linear model, finding a *D*-optimal design involves selecting the *n* design points so that the determinant of the information matrix $\boldsymbol{X}'\boldsymbol{X}$ is maximised, where $\boldsymbol{X}$ is the $n \times p$ model matrix constructed by expanding the design matrix to model form. In linear models, the model matrix and consequently, the $\boldsymbol{X}'\boldsymbol{X}$ matrix contains only functions of the design points. Generalised linear models are non-linear models and the *D*-optimal design must be chosen to maximise the determinant of the asymptotic information matrix $\boldsymbol{X}'\boldsymbol{V}\boldsymbol{X}$, where $\boldsymbol{V}$ is the $n \times n$ diagonal matrix of weights that depends on the specific generalised linear model that has been used. For equation (2), the logistic regression model, the diagonal elements of $\boldsymbol{V}$ are

$$V_{ii} = \frac{e^{\boldsymbol{x}_i'\boldsymbol{\beta}}}{\left(1 + e^{\boldsymbol{x}_i'\boldsymbol{\beta}}\right)^2} \tag{4}$$

and for the Poisson model

$$V_{ii} = e^{\boldsymbol{x}_i'\boldsymbol{\beta}} \tag{5}$$

Because the information matrix $\boldsymbol{X}'\boldsymbol{V}\boldsymbol{X}$ contains the unknown model parameters $\boldsymbol{\beta}$, the usual approach to finding a *D*-optimal design for a linear model will not work. In general, the covariance matrix for any non-linear model will contain the unknown model parameters.

Box and Lucas (1959) have applied the *D*-criterion to find designs for non-linear regression models. There are reviews of designs for non-linear models in Ford et al. (1989) and Atkinson et al. (2007). Chernoff (1953) proposed choosing values for the unknown model parameters and finding the design that maximised the determinant of the covariance for this specific set of parameters. This leads to the idea of a local *D*-optimal design. This approach can work well if the estimates of the unknown parameters are close to the actual values. Another approach is to use a sequential design strategy; begin with a design that is smaller than the size of the final design, run this experiment and obtain preliminary estimates of the model parameters, then use these parameter estimates as if they were the true values of the parameters and augment the original design with additional runs to produce the final design.

A Bayesian approach uses a prior distribution $f(\boldsymbol{\beta})$ to specify the uncertainty in the parameter values. This leads to a design criterion

$$\phi = \int \log|\boldsymbol{X}'\boldsymbol{V}\boldsymbol{X}| f(\boldsymbol{\beta})\, d\boldsymbol{\beta} \tag{6}$$

This is the expectation of the logarithm of the determinant of the information matrix. This criterion was proposed by Chaloner and Larntz (1989) for single-factor logistic regression. The difficulty in using equation (6) as a design criterion is that the *p*-dimensional integral must be evaluated a very large number of times. Gotwalt et al.

(2009) have recently developed a novel quadrature scheme that greatly improves the computing time to evaluate the integral in equation (6) and which exhibits excellent numerical accuracy. This procedure is implemented in the non-linear design platform of JMP, and uses a coordinate exchange algorithm as the basis of design construction.

We will use this approach to construct *D*-optimal design for second-order response surface designs for both the logistic and Poisson regression models for k = 2, 3, and 4 design factors. Consider first the case of a logistic regression response surface model with k = 2 factors. Suppose that the prior information on the model parameters can be summarised by a normal distribution with means and $\pm 2\sigma$ limits as follows:

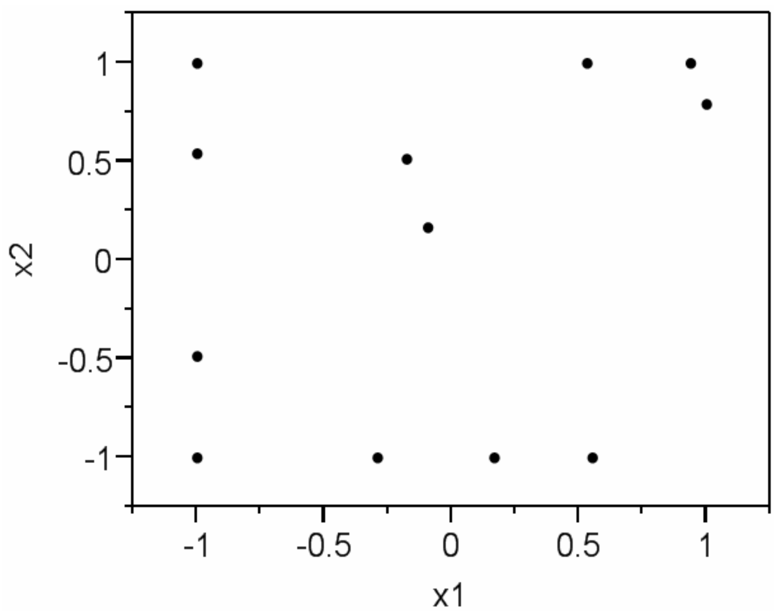
$$\begin{array}{ccccc} 1 & \leq & \beta_0 & \leq & 3 \\ 1.5 & \leq & \beta_1 & \leq & 4.5 \\ -1 & \leq & \beta_2 & \leq & -3 \\ 1.5 & \leq & \beta_{11} & \leq & 4.5 \\ -0.5 & \leq & \beta_{12} & \leq & -1.5 \\ -2 & \leq & \beta_{22} & \leq & -6 \end{array} \tag{7}$$

The 12-run *D*-optimal design from JMP is shown in Table 1 and Figure 1. A logical ‘standard’ 12-run design to compare this design to would be a face-centred cube with four centre runs. The *D*-optimal design has 12 distinct design points where the face-centred cube has only nine, and the *D*-optimal design shares only two points in common with the face-centred cube. The two designs are quite different.

Table 1 A 12-run *D*-optimal second-order design for a logistic regression model with k = 2 using the normal prior in equation (7)

Run	*x1*	*x2*
1	0.52660431	1
2	–0.0961586	0.16409345
3	0.55196771	–1
4	0.94182103	1
5	–1	–0.4836986
6	–1	–1
7	–0.2905524	–1
8	1	0.79805201
9	–0.1779733	0.51622555
10	0.17065821	–1
11	–1	0.5440364
12	–1	1

Figure 1 A 12-run *D*-optimal second-order design for a logistic regression model using the normal prior in equation (7)



Now, consider the case of a logistic regression response surface model with $k = 3$ factors. Suppose that the prior information on the model parameters can be summarised by a normal distribution with means and $\pm 2\sigma$ limits as follows:

$$\begin{array}{rcccl} 1 & \leq & \beta_0 & \leq & 3 \\ 1.5 & \leq & \beta_1 & \leq & 4.5 \\ -1 & \leq & \beta_2 & \leq & -3 \\ 1.5 & \leq & \beta_3 & \leq & 4.5 \\ 1.5 & \leq & \beta_{11} & \leq & 4.5 \\ -2 & \leq & \beta_{22} & \leq & -6 \\ -2 & \leq & \beta_{33} & \leq & -6 \\ -0.5 & \leq & \beta_{12} & \leq & -1.5 \\ -0.5 & \leq & \beta_{13} & \leq & -1.5 \\ -0.5 & \leq & \beta_{23} & \leq & -1.5 \end{array} \tag{8}$$

The 18-run *D*-optimal design that we constructed for this scenario is shown in Table 2. The face-centred cube with four centre points would be a logical standard design to compare to this optimal design. The face-centred cube has 15 distinct design points while the optimal design in Table 2 has no replicates, and it does not share any points in common with the face-centred cube. As we saw in the $k = 2$ case, the optimal design is very different from a comparable standard design with the same number of runs.

Table 2 An 18-run *D*-optimal second-order design for a logistic regression model with $k = 3$ using the normal prior in equation (8)

Run	*x1*	*x2*	*x3*
1	1	0.25099569	–1
2	–1	0.86782641	–0.111647
3	1	–1	–0.6774065
4	–1	0.79028727	1
5	0.97686529	1	1
6	1	0.59129776	1
7	–1	0.2905937	–0.0783575
8	0.82631504	–1	–1
9	0.6240754	–1	1
10	1	0.9309025	–1
11	–0.0101792	–0.2270992	–0.4353463
12	–1	–1	–0.2404986
13	1	1	–0.1553708
14	0.01560598	0.59108721	0.27055434
15	–1	–0.9824465	0.45133389
16	–1	0.01873152	1
17	–1	–0.0726914	–0.6309818
18	–0.1770412	–1	1

The final case that we consider for logistic regression is for $k = 4$ factors. We assume that the prior distribution for the model parameters is normal with means and $\pm 2\sigma$ limits as follows:

$$
\begin{array}{rcccl}
1 & \leq & \beta_0 & \leq & 3 \\
1.5 & \leq & \beta_1 & \leq & 4.5 \\
-1 & \leq & \beta_2 & \leq & -3 \\
1.5 & \leq & \beta_3 & \leq & 4.5 \\
1.5 & \leq & \beta_4 & \leq & 4.5 \\
1.5 & \leq & \beta_{11} & \leq & 4.5 \\
-2 & \leq & \beta_{22} & \leq & -6 \\
-2 & \leq & \beta_{33} & \leq & -6 \\
0.5 & \leq & \beta_{44} & \leq & 1.5 \\
-0.5 & \leq & \beta_{12} & \leq & -1.5 \\
-0.5 & \leq & \beta_{13} & \leq & -1.5 \\
0.5 & \leq & \beta_{14} & \leq & 1.5 \\
-0.5 & \leq & \beta_{23} & \leq & -1.5 \\
1 & \leq & \beta_{24} & \leq & 3 \\
0.5 & \leq & \beta_{34} & \leq & 1.5
\end{array}
\tag{9}
$$

The second-order model for k = 4 factors has 15 parameters. We constructed both an 18-run design and a 28-run design for this model. These designs are shown in Tables 3 and 4 respectively. There is no 'standard' 18-run design to compare to the 18-run optimal design in Table 3 so we constructed an 18-run *D*-optimal design for a normal-theory second-order response surface model using JMP. This design is shown in Table 5. The *D*-optimal design in Table 3 does not share any points in common with this design. A logical standard design to compare to the 28-run design is a face-centred cube with four centre runs. The optimal design in Table 4 does not share any runs in common with the face-centred cube and it does not have any replicates. The face-centred cube has 25 distinct design points.

Table 3 An 18-run *D*-optimal second-order design for a logistic regression model with k = 4 using the normal prior in equation (9)

Run	*x1*	*x2*	*x3*	*x4*
1	–1	1	–0.3363465	0.99348799
2	0.45267715	–0.9391371	–0.7879299	0.32836793
3	–1	0.19250867	–0.3824655	–1
4	–0.9009019	0.70049754	0.93145648	0.24578529
5	0.81057841	–1	–0.8042694	1
6	–0.5243816	–1	0.26722678	1
7	–1	–0.4940153	0.58633327	–1
8	0.32453861	0.69716532	–0.8952356	1
9	1	0.12937652	–0.8938286	–1
10	0.99617027	0.9955783	–0.0877292	–0.1810068
11	0.03493221	0.23251933	0.36978483	–1
12	1	0.30859526	1	–0.8050969
13	0.27984215	0.92497963	1	0.90649769
14	0.46444282	–1	–0.4516155	–1
15	–0.1357471	–0.042767	–0.2318467	–0.0237575
16	–1	–0.5058793	–0.5341066	1
17	0.04918482	–1	1	–0.0600287
18	–1	–0.9927485	–0.1590322	–1

Table 4 A 28-run *D*-optimal second-order design for a logistic regression model with $k = 4$ using the normal prior in equation (9)

Run	*x1*	*x2*	*x3*	*x4*
1	–1	1	–0.2986801	0.77642356
2	–1	–1	–0.4277555	–1
3	–1	–0.0257634	–0.6122526	0.16880807
4	–0.1529687	1	1	–1
5	1	0.30033218	–0.8961585	–1
6	–0.1028279	1	1	1
7	0.92285744	0.86082361	0.5166954	–1
8	–1	0.52432952	0.96863738	0.2513297
9	–0.1992239	–1	–0.2964621	1
10	–1	–0.9521252	0.4319682	–1
11	0.34805939	0.3208145	–1	1
12	–0.0686026	0.21083069	–0.1185675	–0.2036811
13	0.6848592	–1	–0.9198524	–1
14	–0.0264656	–1	1	1
15	0.22814041	–1	1	–1
16	–1	0.7274504	–0.3455637	0.78861117
17	–1	1	–0.3092668	–1
18	0.84729468	0.44784216	1	0.12152886
19	–1	0.14556659	–0.2487869	–1
20	0.98082583	1	–0.5931724	0.32152327
21	1	1	1	0.0349432
22	0.88574221	–1	–0.916611	0.77818126
23	–1	0.53356433	1	–1
24	–1	–0.4184638	–0.432	1
25	–0.8563488	–1	1	0.35430086
26	–1	–1	–0.4080704	–1
27	0.66478864	–0.9144135	–0.3335624	–1
28	1	–1	1	–0.9944456

Table 5 An 18-run *D*-optimal design for second-order linear model with $k = 3$

Run	*x1*	*x2*	*x3*	*x4*
1	1	–1	0	–1
2	1	1	–1	1
3	1	1	1	–1
4	–1	1	–1	1
5	–1	–1	0	1
6	0	–1	–1	–1
7	1	–1	–1	1
8	–1	1	1	1
9	–1	1	–1	–1
10	0	1	0	0
11	1	1	–1	–1
12	–1	–1	–1	0
13	0	0	–1	1
14	1	1	1	1
15	1	0	1	0
16	0	–1	1	1
17	–1	0	0	–1
18	–1	–1	1	–1

We now consider the case of a Poisson regression response surface model with $k = 2$ factors. Suppose that the prior information on the model parameters can be summarised by a normal distribution with means and $\pm 2\sigma$ limits as follows:

$$\begin{array}{rcccl} 1 & \leq & \beta_0 & \leq & 3 \\ 10.25 & \leq & \beta_1 & \leq & 0.75 \\ -0.1 & \leq & \beta_2 & \leq & -0.3 \\ 0.45 & \leq & \beta_{11} & \leq & 1.35 \\ -0.2 & \leq & \beta_{12} & \leq & -0.6 \\ -0.2 & \leq & \beta_{22} & \leq & -0.6 \end{array} \tag{10}$$

The 12-run *D*-optimal design from JMP is shown in Table 6 and Figure 2. A logical 'standard' 12-run design to compare this design to would be a face-centred cube with four centre runs. The *D*-optimal design has eight distinct design points compared to nine for the face-centred cube, but the *D*-optimal design only shares five points in common with the face-centred cube.

Table 6 A 12-run *D*-optimal second-order design for a Poisson regression model with $k = 2$ using the normal prior in equation (10)

Run	*x1*	*x2*
1	–1	–0.1510261
2	–1	1
3	0.48006024	–1
4	1	–1
5	1	1
6	1	1
7	1	–1
8	–1	–1
9	–1	1
10	0.34793736	–0.2587646
11	1	–0.2330349
12	1	–0.2330349

Figure 2 A 12-run *D*-optimal second-order design for a Poisson regression model with $k = 2$ using the normal prior in equation (7)

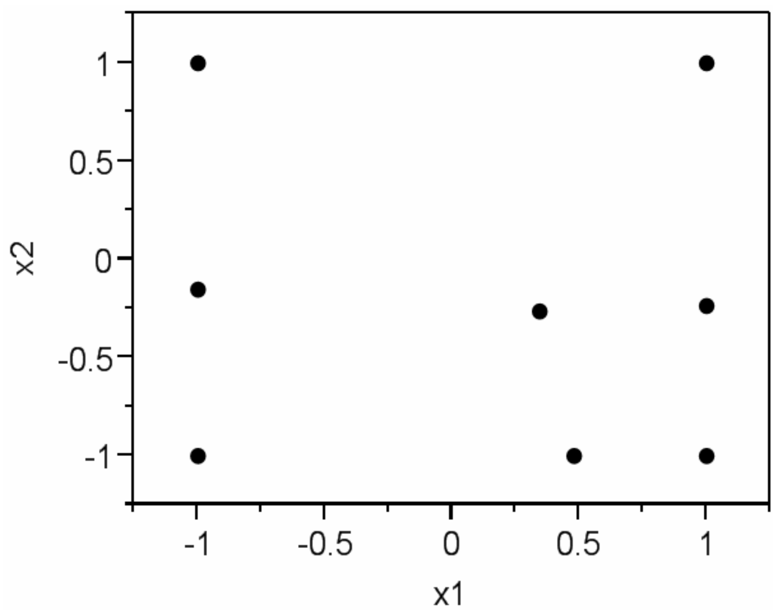


Table 7 shows the 18-run design for the Poisson regression response surface model with $k = 3$ factors and a normal prior distribution specified as follows:

$$\begin{array}{rcccl} 1 & \le & \beta_0 & \le & 3 \\ 0.25 & \le & \beta_1 & \le & 0.75 \\ -0.1 & \le & \beta_2 & \le & -0.3 \\ 0.5 & \le & \beta_3 & \le & 1.5 \\ 0.45 & \le & \beta_{11} & \le & 1.35 \\ -0.2 & \le & \beta_{22} & \le & -0.6 \\ -0.25 & \le & \beta_{33} & \le & 0.75 \\ -0.5 & \le & \beta_{12} & \le & -1.5 \\ 0.25 & \le & \beta_{13} & \le & 0.75 \\ 0.5 & \le & \beta_{23} & \le & 1.5 \end{array} \tag{11}$$

Once again, we see that there are a number of runs in common with the face-centred cube and four replicated runs.

Table 7 An 18-run D-optimal second-order design for a Poisson regression model with $k = 3$ using the normal prior in equation (11)

Run	*x1*	*x2*	*x3*
1	0.37810329	0.05695444	1
2	1	–1	–1
3	–1	–0.0296346	–1
4	1	–1	1
5	–1	–1	–1
6	1	–1	0.17146872
7	–1	1	–1
8	–1	–0.0959812	1
9	1	1	1
10	1	1	1
11	1	–0.1219659	–1
12	1	–0.1546912	0.38893985
13	0.00067289	1	1
14	1	–1	–1
15	–1	1	1
16	–1	1	1
17	1	–0.0420354	1
18	1	–1	1

Finally, we constructed both an 18-run design and a 28-run design for the second-order model for $k = 4$ factors. These designs are shown in Tables 8 and 9 respectively. Recall that there is no ‘standard’ 18-run design to compare to the 18-run optimal design in Table 8 so we will use the 18-run *D*-optimal design for a normal-theory second-order model from JMP, shown previously in Table 5. The 28-run design is compared to a face-centred cube with four centre runs. The normal prior on the parameters and the prior information on the model parameters is as follows and the designs are shown in Table 8 and Table 9.

$$\begin{array}{ccccc} 1 & \leq & \beta_0 & \leq & 3 \\ 0.25 & \leq & \beta_1 & \leq & 0.75 \\ -0.1 & \leq & \beta_2 & \leq & -0.3 \\ 0.5 & \leq & \beta_3 & \leq & 1.5 \\ 0.5 & \leq & \beta_4 & \leq & 1.5 \\ 0.45 & \leq & \beta_{11} & \leq & 1.35 \\ -0.2 & \leq & \beta_{22} & \leq & -0.6 \\ 0.25 & \leq & \beta_{33} & \leq & 0.75 \\ 0.25 & \leq & \beta_{44} & \leq & 0.75 \\ -0.5 & \leq & \beta_{12} & \leq & -1.5 \\ 0.25 & \leq & \beta_{13} & \leq & 0.75 \\ 0.125 & \leq & \beta_{14} & \leq & 0.375 \\ 0.5 & \leq & \beta_{23} & \leq & 1.5 \\ 0.25 & \leq & \beta_{24} & \leq & 0.75 \\ -0.25 & \leq & \beta_{34} & \leq & -0.75 \end{array} \tag{12}$$

Table 8 A 18-run *D*-optimal second-order design for a Poisson regression model with $k = 4$ using the normal prior in equation (12)

Run	*x1*	*x2*	*x3*	*x4*
1	–1	1	1	–1
2	1	–1	–1	–1
3	–1	1	1	0.230603
4	1	–1	–1	1
5	–1	1	–1	1
6	1	1	1	–1
7	1	0.052321	1	1
8	–1	1	1	1
9	1	1	1	1
10	1	–1	–1	0.322907
11	–1	–0.87965	–1	1
12	1	–1	1	1
13	0.111111	1	1	1
14	1	–0.77832	0.077451	1
15	1	–1	1	–1
16	–1	0.192072	1	1
17	1	0.090304	–1	1
18	1	–0.03498	1	–1

Table 9 A 28-run *D*-optimal second-order design for a Poisson regression model with $k = 4$ using the normal prior in equation (12)

Run	*x1*	*x2*	*x3*	*x4*
1	1	1	1	–1
2	1	–1	–1	–1
3	–1	–0.8367479	–1	1
4	1	–1	–0.0084293	1
5	1	1	1	1
6	1	0.03760119	1	1
7	1	0.07620255	0.32317288	1
8	0.11112387	1	1	1
9	–1	1	1	1
10	1	–1	1	1
11	1	1	1	1
12	1	–1	1	1
13	–1	1	1	–1
14	1	–0.0754533	1	–1
15	–1	–0.1834005	1	–1
16	1	–1	1	–1
17	0.11110748	1	1	1
18	1	–1	–1	–1
19	1	–1	–1	1
20	–1	1	1	–1
21	1	0.13852609	–1	1
22	1	–1	1	–0.0032746
23	1	0.22289572	1	0.30628991
24	–1	1	–1	1
25	1	–1	–1	1
26	–1	0.18573968	1	1
27	–1	1	1	1
28	–1	1	1	0.24602819

3 Efficiency of standard designs

We have observed that the *D*-optimal response surface design for a generalised linear model can differ quite a bit from a response surface standard design, such as a face-centred cube. It is of interest to more formally compare the D-optimal design with the standard design. We will do this using a measure of design efficiency based on the design criterion in equation (6). Specifically, for a particular scenario (type of generalised linear model, prior distribution, and design), we will use Monte Carlo methods to randomly sample 1,000 times from the prior distribution for that scenario and for each choice of the parameter vector evaluate $\log|\boldsymbol{X'VX}|$ for the standard design and the D-optimal design to produce a local efficiency at that set of prior parameters. The average of these $\log|\boldsymbol{X'VX}|$ values for each design is an approximation of the integral in equation (6). We take as the efficiency of the standard response surface design relative to the D-optimal design the ratio

$$E = e^{\frac{\sum_{i=1}^{1000} \log|\boldsymbol{X'V}_i\boldsymbol{X}|_{Factorial} - \sum_{i=1}^{1000} \log|\boldsymbol{X'V}_i\boldsymbol{X}|_{D-optimal}}{1000p}} \tag{13}$$

where p is the number of parameters in the model. Values of this ratio that are less than unity indicate that the standard design is less efficient than the D-optimal design for that particular scenario.

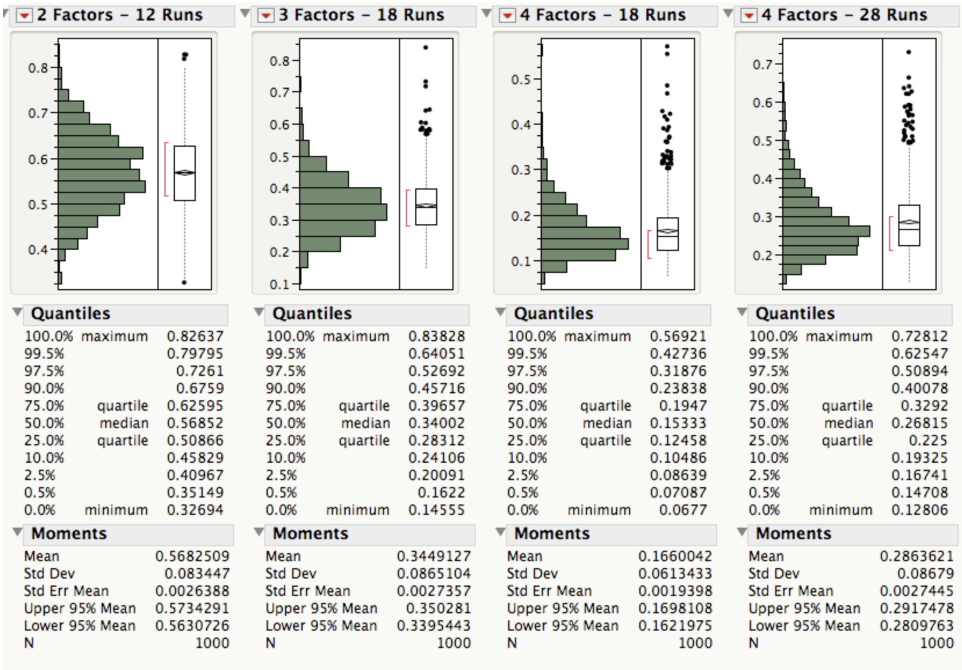
Table 10 shows the average of the local efficiencies for the optimal designs for the logistic and Poisson regression models compared to the standard design choices. The efficiencies vary from about 16% to slightly over 80%, with the standard designs exhibiting higher efficiencies for the Poisson case than for the logistic regression case. The efficiencies for the 18-run D-optimal design for the linear model for $k = 4$ are lower that the efficiencies for the face-centred cube with 28 runs. This is not unexpected, as the 18-run design is nearly saturated and additional runs often improve design efficiency in these situation.

Table 10 Average relative efficiency of a standard response surface design to the D-optimal design for a second-order logistic or Poisson regression model

Factors	*Runs*	*Averaged relative efficiency standard design to D-optimal*	
		Logistic second-order	*Poisson second-order*
2	12	0.561992239	0.816186271
3	18	0.334293209	0.499726763
4	18	0.156658721	0.293492748
4	28	0.274875301	0.362560773

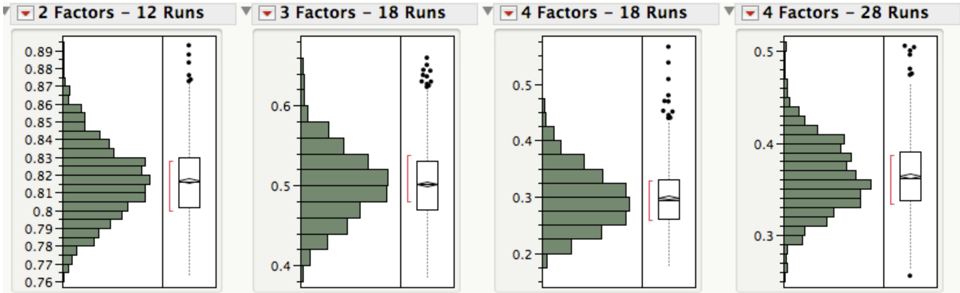
Figures 3 and 4 present the histograms and summary statistics for the local efficiencies for all designs considered. Figure 3 contains the results for the logistic regression model and Figure 4 presents the Poisson regression model results. The histograms indicate that the local efficiencies can vary considerably. For example, in the logistic regression case with $k = 3$, the local efficiencies vary from about 14.5% to over 83%, and in the Poisson regression case with $k = 3$ and $n = 18$, the local efficiencies vary from about 38.5% to almost 66%. Generally, there is less variability in the local efficiencies for the Poisson case than for the logistic regression model (binomial) case. This variability in local efficiency is a reflection of sampling different parameter vectors from the prior distribution. It is interesting to note, and not unexpected, that there are no situations where the local efficiency of the standard design exceeds the local efficiency of the optimal design chosen from that particular response distribution.

Figure 3 Local relative efficiencies of the standard design versus the *D*-optimal logistic regression design (see online version for colours)



Note: All standards designs are face-centred cubes except for $k = 4$ and $n = 18$ where a *D*-optimal design for a linear model was used.

Figure 4 Local relative efficiencies of the standard design versus the *D*-optimal Poisson regression design (see online version for colours)



Quantiles

		2 Factors – 12 Runs	3 Factors – 18 Runs	4 Factors – 18 Runs	4 Factors – 28 Runs
100.0%	maximum	0.8928	0.6596	0.56556	0.50522
99.5%		0.87359	0.63803	0.46948	0.48032
97.5%		0.85877	0.59223	0.41393	0.43901
90.0%		0.84383	0.55847	0.36831	0.41223
75.0%	quartile	0.82974	0.53016	0.33019	0.39122
50.0%	median	0.81615	0.50147	0.29359	0.36238
25.0%	quartile	0.80143	0.47015	0.25995	0.3377
10.0%		0.78934	0.44516	0.2352	0.31775
2.5%		0.77695	0.41949	0.2065	0.29686
0.5%		0.76798	0.39943	0.19206	0.26868
0.0%	minimum	0.76365	0.3848	0.17546	0.25598

Moments

	2 Factors – 12 Runs	3 Factors – 18 Runs	4 Factors – 18 Runs	4 Factors – 28 Runs
Mean	0.8164598	0.5016632	0.2981574	0.3645085
Std Dev	0.0211747	0.0442121	0.0535456	0.037795
Std Err Mean	0.0006696	0.0013981	0.0016933	0.0011952
Upper 95% Mean	0.8177737	0.5044068	0.3014802	0.3668538
Lower 95% Mean	0.8151458	0.4989197	0.2948347	0.3621631
N	1000	1000	1000	1000

Note: All standards designs are face-centred cubes except for $k = 4$ and $n = 18$ where a *D*-optimal design for a linear model was used.

4 An application to plasma etching

Semiconductor wafers usually undergo a series of repeated processing steps, one of which is plasma etching. This is often accomplished in a single-wafer tool in which the factors pressure, anode-cathode gap, and RF power are among those that can be controlled. Sometimes, the mixture of gas species is studied as well, but those components were fixed in this experiment. The objective of the experiment was to reduce and if possible, eliminate surface defects on the wafers that arise during etching. Previous experiments had determined operating conditions on pressure, anode-cathode gap and RF power that resulted in a satisfactory etch rate and near-optimal uniformity of the etched surface. The boundaries on those operating conditions cannot be exceeded, so a face-centred cube would be a reasonable choice of design if a standard design is to be used. However, the experimenter did not want to use this design because the response variable most likely has a Poisson distribution and a generalised linear model is going to be required to model the response. Therefore, an 18-run *D*-optimal design for a second-order Poisson regression model was selected. Based on previous experience with this etching tool and from conducting earlier experiments to study the occurrence of defects, the experimenters selected a normal prior with means and $\pm 2\sigma$ ranges on the parameters as follows:

$$\begin{array}{rcccl} 1 & \leq & \beta_0 & \leq & 4 \\ 0.22 & \leq & \beta_1 & \leq & 0.8 \\ -0.1 & \leq & \beta_2 & \leq & 0.8 \\ 0.5 & \leq & \beta_3 & \leq & -1.5 \\ 0.25 & \leq & \beta_{11} & \leq & 0.75 \\ 0.25 & \leq & \beta_{22} & \leq & 0.75 \\ 0.25 & \leq & \beta_{33} & \leq & 0.75 \\ 0.25 & \leq & \beta_{12} & \leq & 0.75 \\ 0.25 & \leq & \beta_{13} & \leq & 0.75 \\ 0.5 & \leq & \beta_{23} & \leq & 1.5 \end{array}$$

The design is shown in Table 11 and the output from JMP for fitting a Poisson generalised linear model to this data is shown in Table 12. There is no indication of lack-of-fit of the model, but some of the model terms, specifically x_1x_3, x_2x_3 and x_3^2, have large *P*-values. We eliminated these terms and fit the reduced model shown in Table 13. This model is also an excellent fit to the data.

Table 11 The *D*-optimal design for the plasma etching experiment

Run	*x1 = pressure*	*x2 = gap*	*x3 = power*	*y, defects*
1	0.011279	–1	–1	4
2	1	0.298655	1	12
3	0.182845	0.306462	1	6
4	–1	–0.01709	–1	7
5	1	–0.188	–1	22
6	1	1	1	13
7	–1	1	–1	23
8	0.349073	1	0.414667	12
9	–1	–1	–1	2
10	1	1	1	13
11	–1	1	1	11
12	1	1	0.402996	16
13	1	1	–1	27
14	–1	1	1	11
15	1	–1	–1	19
16	1	–1	1	9
17	1	1	–1	27
18	0.26895	1	1	10

Table 12 JMP output for the full second-order Poisson regression model

Generalised linear model fit

Weight	Variance of *Y*
Response	Defects
Distribution	Poisson
Link	Log
Estimation method	Maximum likelihood
Observations (or sum wgts)	1118

Whole model test

Model	*-LogLikelihood*	*L-R ChiSquare*	*DF*	*Prob > ChiSq*
Difference	509.575987	1019.152	9	<.0001*
Full	2387.63589			
Reduced	2897.21187			

Goodness of fit statistic	*ChiSquare*	*DF*	*Prob > ChiSq*
Pearson	2.8272	8	0.9447
Deviance	2.8295	8	0.9446

AICc

4826.7003

Effects tests

Source	*DF*	*L-R ChiSquare*	*Prob > ChiSq*
x1	1	446.37281	< .001*
x2	1	303.05283	< .001*
x3	1	222.51988	< .001*
x1*x1	1	48.306618	< .001*
x1*x2	1	129.62517	< .001*
x2*x2	1	3.1982568	0.0737
x1*x3	1	0.7045149	0.4013
x2*x3	1	0.5858496	0.4440
x3*x3		0.0046547	0.9456

Parameter estimates

Term	*Estimate*	*Std error*	*L-R ChiSquare*	*Prob > ChiSq*	*Lower CL*	*Upper CL*
Intercept	1.8872405	0.0768591	474.4063	< .001*	1.7351659	2.0364974
x1	0.6360931	0.0385066	446.37281	< .001*	0.5625054	0.7135258
x2	0.74147	0.0456714	303.05284	< .001*	0.6530479	0.8321816
x3	–0.377114	0.0219884	222.51988	< .001*	–0.419537	–0.333307
x1*x1	0.2602469	0.0383729	48.306618	< .001*	0.1855693	0.3360036
x1*x2	–0.577428	0.0535283	129.62517	< .001*	–0.683476	–0.473596
x2*x2	–0.045167	0.025224	3.1982568	0.0737	–0.09454	0.0043401
x1*x3	0.0270944	0.0323454	0.7045149	0.4013	–0.036021	0.0908333
x2*x3	0.0225041	0.0295769	0.5858496	0.4440	–0.03459	0.0813652
x3*x3	–0.004839	0.0709066	0.0046547	0.9456	–0.142896	0.1351451

Table 13 JMP output for reduced second-order Poisson regression model

			Generalised linear model fit			
Weight				Variance of *Y*		
Response				Defects		
Distribution				Poisson		
Link				Log		
Estimation method				Maximum likelihood		
Observations (or sum wgts)				1118		
			Whole model test			
Model	*-LogLikelihood*		*L-R ChiSquare*	*DF*	*Prob > ChiSq*	
Difference	509.154603		1018.309	6	<.0001*	
Full	2388.05727					
Reduced	2897.21187					
Goodness of fit statistic	*ChiSquare*		*DF*		*Prob > ChiSq*	
Pearson	3.6651		11		0.9787	
Deviance	3.6722		11		0.9785	
AICc						
4801.3145						
			Effects tests			
Source	*DF*		*L-R ChiSquare*		*Prob > ChiSq*	
x1	1		446.01513		< .001*	
x2	1		542.36627		< .001*	
x3	1		594.94919		< .001*	
x1*x1	1		53.37396		< .001*	
x1*x2	1		296.14918		< .001*	
x2*x2	1		2.830613		0.0925	
			Parameter estimates			
Term	*Estimate*	*Std error*	*ChiSquare*	*Prob > ChiSq*	*Lower CL*	*Upper CL*
Intercept	1.8949772	0.0449511	1045.4678	< .001*	1.8058067	1.9820546
x1	0.6307513	0.0379366	466.01513	< .001*	0.5583088	0.7071012
x2	0.7302926	0.0398101	542.36627	< .001*	0.6540568	0.8101906
x3	–0.367087	0.0143953	594.94919	< .001*	–0.395217	–0.338786
x1*x1	0.2661641	0.0374249	53.37396	< .001*	0.1933563	0.3400761
x1*x2	–0.546541	0.0390759	296.14918	< .001*	–0.625142	–0.471887
x2*x2	–0.039879	0.0236517	2.830613	0.0925	–0.086122	0.0065949

Figures 5 and 6 present the prediction profiler and contour plot from JMP for the reduced model. From examining these plots, it is apparent that operating this process in the vicinity of low pressure, small gap and high power presents the best opportunity for defect reduction. Because the operating conditions are near the extremes of the region, one might be tempted to conduct further experiments outside of these boundaries. However, it has been established that operating outside of this region leads to unacceptable etch rate and uniformity.

Figure 5 Contour profile plots from JMP (see online version for colours)

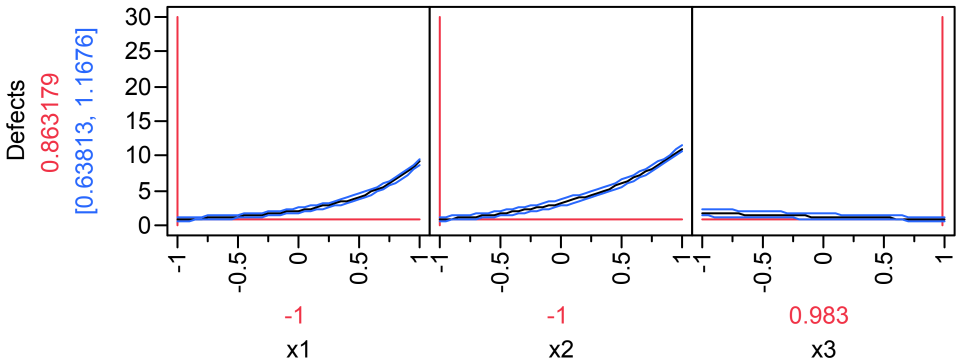
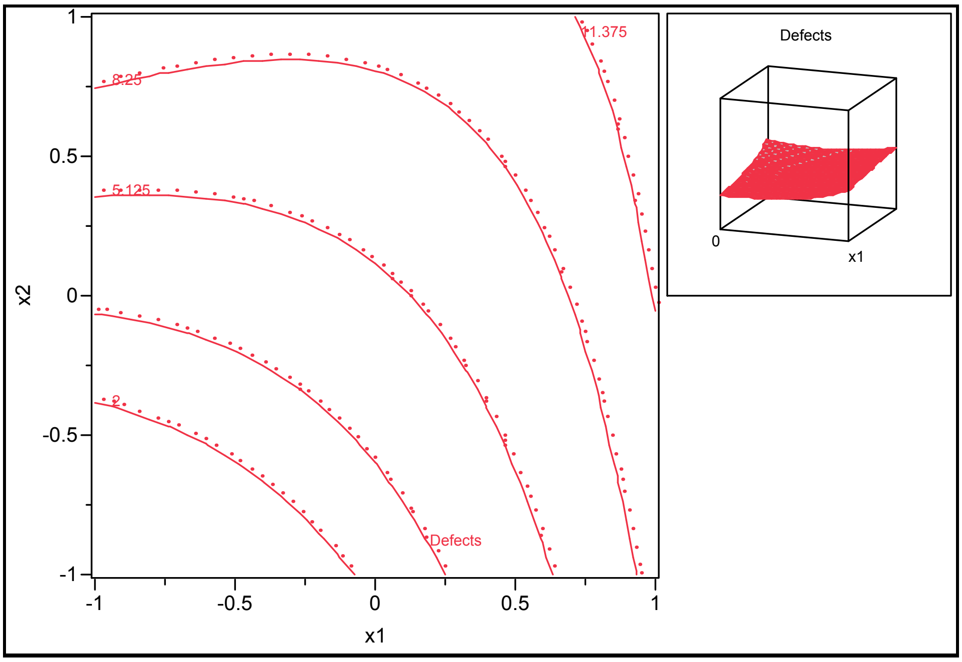


Figure 6 Contour plot from JMP with x1 = 1 (see online version for colours)



5 Conclusions

We have demonstrated that modern computer software implementation of the Bayesian criterion makes it relatively straightforward to generate *D*-optimal designs for generalised linear models. For two specific cases, second-order response surface models involving logistic and Poisson regression, we have shown that a standard design choice has relatively low efficiency in comparison to the *D*-optimal design. We also showed that a *D*-optimal design for a second-order response model and a logistic regression model was superior to a *D*-optimal design for a linear model with a second-order polynomial in the exponent when that design was used to fit the generalised linear model. While our study is limited, we suspect that in many situations, these optimal designs will significantly outperform standard designs when fitting generalised linear models. We have developed a relatively straightforward procedure to evaluate the efficiency of these comparisons.

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