Locally D-optimal design for weighted exponential model and its computation

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Abstract. Weighted exponential model is used as a growth curve. We introduce locally D-optimal design for weighted exponential model with three parameters. The assumption of this model is homoscedastic error. D-optimal criterion is a criterion which is the value of standardized variance less than or same the number of parameters. The design in this paper, number of supported design is three and have same weight. Determination of the supported designs by maximizing the determinant of the information matrix. We present this formula, this is a nonlinear model, so to maximizing it we use numerically approach.

1. Introduction

In conducting research after the model is established, the problem is how to choose supported design must be run so that it meets the optimal criteria. In this paper, the D-optimal criterion is used. D-optimal criterion is optimality with the aim to minimize the variance of the parameters estimator so that the parameters in the model are significant. Determination of supported designs that meet the D-optimality by maximizing the determinant of the information matrix. D-optimality criterion can be applied both on linear and nonlinear models. Polynomial regression model is a linear model, D-optimal design for this model is do, they are \([1,2,3]\) for the homoscedastic cases. While in heteroscedastic, they are \([4,5]\).

Kiefer and Wolfowitz \([6]\) found that G-optimal and D-optimal are equivalent. This theorem is known as the Equivalence Theorem, and this theorem will be used to prove that the supported designs satisfy the D-optimal criterion. D-optimal design also depends on the model which we used. In nonlinear models the determination of D-optimal design becomes complicated. This is because the information matrix in the nonlinear model contains an unknown parameter so needs information of the value of the parameter.

The weighted exponential distribution function has a specific curve shape, the curve from zero reaches the maximum point then down, and at a certain time it is relatively constant closed to zero. This function can be used to describe the growth curve model. Gupta and Kundu \([7]\) introduced the weighted exponential (WE) distribution as an alternative to Gamma or Weibull distribution. The distribution function of weighted exponentials is:

\[
f(x) = \frac{1+\theta_2}{\theta_2} \theta_1 e^{-\theta_1 x} \left(1 - e^{-\theta_1 \theta_2 x}\right), \quad x > 0, \quad \theta_1, \theta_2 > 0
\]

The curve of model (1) has a maximum point at \(x = \frac{\ln(1+\theta_2)}{\theta_1 \theta_2}\). Model in equation (1) is a nonlinear model.
D-optimal design for nonlinear model has been studied in both homoskedastic and heteroskedastic cases. The models are used for different applications. In the homoskedastic case [8] developed a model which is the form of multiplication between exponential with polynomials of degree \( n \). Hans and Chaloner [9] used an exponential model that was applied to pharmacokinetics, and the logarithm of the exponential model applied to plasma HIV RNA. Dette et al. [10] used four types of exponential models; the first model was applied in agriculture and called the Mitscherlich's growth model, the second and third models were applied for legume growth analysis, and the fourth model was applied in the field of pharmacokinetics. Dette and Pepelyshev [11] used sigmoid model. Atkinson [12] used an exponential model that is applied in the healthy field, which is determining the concentration of drugs in the blood. Widiharih et al. [13] developed an exponential model with mean weighted into a weight exponential model with two parameters and a generalized exponential model with two parameters. Widiharih et al. [14] introduced locally D-optimal designs for Morgan Mercer Flodin (MMF) with three parameters.

Based on the equation (1), we construct design for the three-parameter weighted exponential that fulfills D-optimality as follows:

\[
y = \theta_3 e^{-\theta_1 x}(1 - e^{-\theta_2 x}) + \varepsilon, \quad x \geq 0, \theta_1, \theta_2, \theta_3 > 0
\]

with homoskedastic errors assumption.

Determination of the D-optimal design of the model (2) by maximizing the determinant of information matrix. We meet with the formula of determinant of information matrix of model (2). This formula is a nonlinear model, then maximize the formula using a numerical approach by Modified Newton method, computation is carried out with MATLAB.

### 2. Preliminaries.

Consider the nonlinear model:

\[
y = \eta(x, \theta) + \varepsilon
\]

with independent \( \varepsilon \sim N(0, \sigma^2) \)

\[
E(Y|x) = \eta(x, \theta)
\]

Designs of \( p \) point supported design is denoted by:

\[
\xi = (x_1, x_2, \ldots, x_p, w_1, w_2, \ldots, w_p)
\]

where: \( w_i = \frac{r_i}{n} \), \( r_i \) : number of observations of the supported design \( x_i \) and \( n = \sum_{i=1}^{p} r_i \), \( \sum_{i=1}^{p} w_i = 1 \).

The information matrix of design \( \xi \) for model (4) is:

\[
M(\xi, \theta) = \sum_{i=1}^{p} w_i h(x_i, \theta)h^T(x_i, \theta)
\]

where \( h(x, \theta) = \left( \frac{\partial \eta(x, \theta)}{\partial \theta} \right) = \left( h_1(x, \theta), h_2(x, \theta), \ldots, h_k(x, \theta) \right)^T \) is the vector of partial derivatives of the conditional expectation \( E(Y|x) \) with respect to the parameters \( \theta \). \( M(\xi, \theta) \) is \( k \times k \) (\( k \) : number of parameters) symmetric matrix. A D-optimal design maximizes \( |M(\xi, \theta)| \), which is the determinant of the information matrix. The standardized variance \( d(\xi, x) \) is:

\[
d(\xi, x) = h^T(x, \theta)M^{-1}(\xi, \theta)h(x, \theta)
\]

The Equivalence Theorem as follows: if a design \( \xi^* \) satisfies any one of the following three conditions, then it satisfies all three:

1. \( \xi^* \) maximizes \( |M(\xi, \theta)| \)
2. \( \xi^* \) minimizes \( \max_x d(\xi, x) \)
3. \( \max_x d(\xi^*, x) = k \)

The Equivalence Theorem can be written as follows:

\[
\xi^* \text{ is D-optimal design } \iff d(\xi^*, x) \leq k
\]

### 3. Results and Discussions

Consider model (2):

\[
y = \theta_3 e^{-\theta_1 x}(1 - e^{-\theta_2 x}) + \varepsilon, \quad x \geq 0, \theta_1, \theta_2, \theta_3 > 0
\]
Model (2) has a unimodal curve, the maximum point occurs at point $x = \frac{\ln(1 + \theta_2)}{\theta_1}$. The curve of model (2) for $\theta_3 = 73.1146$; $\theta_1 = 0.07119$ at several of $\theta_2$ 0.1561; 0.1661; 0.1761; 0.1861; 0.1961 and for $\theta_3 = 73.1146$; $\theta_2 = 0.1561$ at several of $\theta_1$ 0.07119; 0.17119; 0.27119; 0.37119; 0.47119 are presented in Figure 1 and Figure 2.

![Figure 1. The curve of model (2) for $\theta_3 = 73.1146$; $\theta_1 = 0.07119$ at several of $\theta_2$](image1)

![Figure 2. The curve of model (2) for $\theta_3 = 73.1146$; $\theta_2 = 0.1561$ at several of $\theta_1$](image2)

Based on Figure 1, if $\theta_3$ and $\theta_1$ fixed and several of $\theta_2$ is closer, then each curve has maximum relatively the same. Based on Figure 2, if $\theta_3$ and $\theta_2$ fixed and several of $\theta_1$ is closer and small, then each curve has different maximum.

Based on model (2) then:

$$
\eta(x, \theta) = \theta_3 e^{-\theta_1 x} (1 - e^{-\theta_2 x})
$$

(8)

Derivatives of $\eta(x, \theta)$ with respect to the parameters $\theta$ is:

$$
\mathbf{h}(x, \theta) = \frac{\partial \eta(x, \theta)}{\partial \theta} = 
\begin{pmatrix}
-\theta_3 xe^{-\theta_1 x} (1 - e^{-\theta_2 x}) \\
\theta_3 xe^{-(\theta_1 + \theta_2)x} \\
x e^{-\theta_1 x} (1 - e^{-\theta_2 x})
\end{pmatrix}
$$

(9)

The information matrix is:

$$
\mathbf{M}(\xi, \theta) =
\begin{pmatrix}
m_{11} & m_{12} & m_{13} \\
m_{12} & m_{22} & m_{23} \\
m_{13} & m_{23} & m_{33}
\end{pmatrix}
$$

(10)

We used design with three points and have the same weight, as follows:

$$
\xi = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}
\begin{pmatrix}
1 \\ 3 \\ 3 \\
1 \\ 3 \\ 3 \\
1 \\ 3 \\ 3
\end{pmatrix}
$$

(11)

The elements of the information matrix are:

$$
m_{11} = \frac{1}{3} \sum_{i=1}^{3} \theta_3^2 x_i^2 e^{-2\theta_1 x_i} (1 - e^{-\theta_2 x_i})^2
$$

$$
m_{22} = \frac{1}{3} \sum_{i=1}^{3} \theta_3^2 x_i e^{-2(\theta_1 + \theta_2) x_i}
$$

$$
m_{33} = \frac{1}{3} \sum_{i=1}^{3} \theta_3 x_i^2 e^{-2\theta_1 x_i} (1 - e^{-\theta_2 x_i})^2
$$

$$
m_{12} = \frac{1}{3} \sum_{i=1}^{3} -\theta_3^2 x_i^2 e^{-2(\theta_1 + \theta_2) x_i} (1 - e^{-\theta_2 x_i})
$$

$$
m_{13} = \frac{1}{3} \sum_{i=1}^{3} -\theta_3 x_i e^{-2\theta_1 x_i} (1 - e^{-\theta_2 x_i})^2
$$
The determinant of the information matrix is:
\[
M_{23} = \frac{1}{3} \sum_{i=1}^{3} \theta_3 x_i e^{-(2\theta_1 + \theta_2)x_i} (1 - e^{-\theta_2 x_i})
\]

The determinant of the information matrix is:
\[
|M(\xi, \theta)| = m_{11} m_{22} m_{33} + 2m_{12} m_{23} m_{13} - m_{22} m_{13}^2 - m_{33} m_{12}^2 - m_{11} m_{23}^2
\]

We have the general formula of the determinant of the information matrix of the model (2) as follows:
\[
|M(\xi, \theta)| \propto e^{-2\theta_1} \sum_{i=1}^{x}[A + B]
\]

where:
\[
A = \sum_{i=1}^{x} (x_i x_j)^2 (1 - e^{-\theta_2 x_k})^2 (e^{-\theta_2 x_i} - e^{-\theta_2 x_j})^2, i \neq j \neq k, k = 2,3
\]
\[
B = 2 \sum_{i=1}^{x^2} x_i x_j x_k (1 - e^{-\theta_2 x_k})(1 - e^{-\theta_2 x_i})(e^{-\theta_2 x_i} - e^{-\theta_2 x_j})(e^{-\theta_2 x_k} - e^{-\theta_2 x_j}), i \neq j \neq k, j = 2,3, k = 1,2,3
\]

Supported designs are maximized \(|M(\xi, \theta)|\) in equation (12). Maximizing \(|M(\xi, \theta)|\) in equation (12) is very difficult and complicated, so we used MATLAB, the program in appendix A1 (define the \(|M(\xi, \theta)|\)), appendix A2 (determine the supported designs and construct the \(M^{-1}(\xi, \theta)\)). Supported designs must satisfy the Equivalence Theorem in equation (7), it needs a program to solve this problem (appendix A3).

For numerical approach with some values of \(\theta_1, \theta_2, \theta_3\), design regions and supported designs of model (2) are presented in Table 1. The supported design in Table 1 fulfill the D-optimallity criterion appropriate with the design region and the information of \(\theta_1, \theta_2, \theta_3\).

| \(\theta_1\)  | \(\theta_2\)  | \(\theta_3\) | Design region | Supported design |
|-----------|-------------|-------------|--------------|-----------------|
| 0.05      | 0.025       | 1           | [0 ,75)      | 7.5053          |
|           |             | 1           | [7.65 ,65)   | 7.600           |
|           |             | 1           | [7.6, 65]    | 7.3717          |
|           |             | 1           | [8 , 55]     | 8.0000          |
| 0.04      | 0.065       | 1           | [0 , 80)     | 6.5366          |
|           |             | 1           | [6, 65]      | 6.5366          |
|           |             | 1           | [7 , 75]     | 7.0000          |
|           |             | 1           | [5, 60]      | 6.5259          |
|           |             | 1           | [7.5, 55]    | 7.5000          |

4. Conclusion
Minimally supported design with uniform weight for each supported design is a simple design, but the information matrix for nonlinear model is more difficult. Formula of determinant information matrix for weighted exponential model is complicated, so that to handle it we use numerical approach with modified Newton by Matlab program. The Equivalence Theorem of Kiefer and Wolfowitz (1960) is used to prove that the design is D-optimal design.

References
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Appendix.

Appendix A1.

MATLAB program to define the $|M(\xi, \theta)|$

```matlab
function f=we3(x,a,b,c)
    x1=x(1);
    x2=x(2);
    x3=x(3);
    a=......;  % insert the information value of a
    b=......;  % insert the information value of b
    c=......;  % insert the information value of c
    k1=(x1*x2)^2*exp(-2*a*(x1+x2+x3))*(1-exp(-b*x3))^2*exp(-2*b*x1*(-b*x2))^2;
    k2=(x1*x3)^2*exp(-2*a*(x1+x2+x3))*(1-exp(-b*x3))^2*exp(-2*b*x1*(-b*x2))^2;
    k3=(x3*x2)^2*exp(-2*a*(x1+x2+x3))*(1-exp(-b*x1))^2*exp(-2*b*x3*(-b*x2))^2;
    k4=(2*x1*x3)*x2^2*exp(-2*a*(x1+x2+x3))*(1-exp(-b*x1))*(1-exp(-b*x2))*(1-exp(-2*b*x2))-exp(-b*x3))^2*(exp(-b*x3)-exp(-b*x1));
    k5=(2*x1*x3)^2*exp(-2*a*(x1+x2+x3))*(1-exp(-b*x1))*(1-exp(-b*x3))*(1-exp(-b*x2))*(1-exp(-2*b*x2))*exp(-b*x3)-exp(-b*x1))^2*(exp(-b*x3)-exp(-b*x1));
    k6=(2*x3*x2)^2*exp(-2*a*(x1+x2+x3))*(1-exp(-b*x3))*(1-exp(-b*x2))*(1-exp(-2*b*x2))*exp(-b*x3)-exp(-b*x1))^2*(exp(-b*x3)-exp(-b*x1));
    det=k1+k2+k3+k4+k5+k6;
    f=det
```

Appendix A2.

MATLAB program to determine supported designs and construct $M^{-1}(\xi, \theta)$

```matlab
function makswe3
    a=......;  % insert the information value of a
    b=......;  % insert the information value of b
    c=......;  % insert the information value of c
    Lb=[......];  % insert lower bound of a,b,c
    Ub=[......];  % insert upper bound of a,b,c
    x0=[......];  % insert initial point of x1, x2 and x3 for iteration processes
    options = optimset('LargeScale','off','GradObj','on','GradConstr','off','TolCon',0.000000001,'TolX',0.000000001)
    [x,nilaimaximum,ExitFlag,output]=fmincon('we3',x0,[],[],[],[],Lb,Ub,[],options)
    x1=x(1);
    x2=x(2);
    x3=x(3);
    m11=0.333333*x^2*(x1^2*exp(-2*a*x1))*(1-exp(-b*x1))^2+x^2*exp(-2*a*x2)*(1-exp(-b*x2))^2+x^2*exp(-2*a*x3)*(1-exp(-b*x3))^2;
    m12=0.333333*x^2*(x1^2*exp(-2*a*x1))*(1-exp(-b*x1))^2+x^2*exp(-2*a*x2)*(1-exp(-b*x2))^2+x^2*exp(-2*a*x3)*(1-exp(-b*x3))^2;
    m13=0.333333*x^2*(x1^2*exp(-2*a*x1))*(1-exp(-b*x1))^2+x^2*exp(-2*a*x2)*(1-exp(-b*x2))^2+x^2*exp(-2*a*x3)*(1-exp(-b*x3))^2;
    m22=0.333333*x^2*(x1^2*exp(-2*a*x1))*(1-exp(-2*a*x2))*(1-exp(-b*x3))^2+x^2*exp(-2*a*x2)*(1-exp(-b*x3))^2+x^2*exp(-2*a*x3)*(1-exp(-b*x3))^2;
    m23=0.333333*x^2*(x1^2*exp(-2*a*x1))*(1-exp(-2*a*x2))*(1-exp(-b*x3))^2+x^2*exp(-2*a*x2)*(1-exp(-b*x3))^2+x^2*exp(-2*a*x3)*(1-exp(-b*x3))^2;
```
\[ m_{33} = 0.33333 \left( \exp(-2a*x1) \right)^2 + \exp(-2a*x2) \right)^2 + \exp(-2a*x3) \right)^2; \]

\[
M = \begin{bmatrix}
m_{11} & m_{12} & m_{13} \\
m_{12} & m_{22} & m_{23} \\
m_{13} & m_{23} & m_{33}
\end{bmatrix}
\]

\[
inves = \text{inv}(M)
\]

\[
save \text{inwe3} \text{ inves}
\]

Appendix A3
Matlab program to determine \( d(\xi, x) \)

\[
\text{function} \ gwe3
\]
\[
syms \ x
\]
\[
inves = \text{load}(\text{'inwe3.mat'});
\]
\[
d1 = \text{struct2cell}(inves);
\]
\[
d2 = \text{cell2mat}(d1);
\]
\[
a = \ldots; \quad \% \text{insert the information value of } a
\]
\[
b = \ldots; \quad \% \text{insert the information value of } b
\]
\[
c = \ldots; \quad \% \text{insert the information value of } c
\]
\[
a1 = -c*x*\exp(-a*x)*(1-\exp(-b*x));
\]
\[
a2 = c*x*\exp(-(a+b)*x);
\]
\[
a3 = \exp(-a*x)*(1-\exp(-b*x));
\]
\[
d3 = [a1 \ a2 \ a3]*d2*[a1; a2; a3];
\]
\[
\text{ezplot}(d3, [2, 35])
\]
\[
\text{grid on}
\]