An algorithm for calculating $D$-optimal designs for polynomial regression with prior information and its applications

Hiroto Sekido

Department of Applied Mathematics and Physics, Graduate School of Informatics, Kyoto University, Kyoto 606-8501, Japan.

Abstract: Optimal designs are required to make efficient statistical experiments. $D$-optimal designs for some models are calculated by using canonical moments. On the other hand, integrable systems are dynamical systems whose solutions can be written down concretely. In this paper, polynomial regression models with prior information are discussed. In order to calculate $D$-optimal designs for these models, a useful relationship between canonical moments and discrete integrable systems is used. By using canonical moments and discrete integrable systems, an algorithm for calculating $D$-optimal designs for these models is proposed. Then some examples of applications of the algorithm are introduced.

Key words: $D$-optimal design, canonical moment, polynomial regression model, discrete integrable system, nonautonomous discrete time Toda equation

1 Introduction

In statistics, design of experiments is a methodology to make efficient experiments. Optimal designs have been studied by numerous authors in the literature. Especially $D$-optimal designs have been investigated by many authors. One of the approaches for $D$-optimal designs is to use canonical moments.

$D$-optimal designs and $D_s$-optimal designs for polynomial regression models were studied in [18]. In the calculation in [18], an important point is to use canonical moments instead of ordinary moments, and $D$-optimal designs can be identified by its canonical moments. As we see in Section 2

\footnote{sekido@amp.i.kyoto-u.ac.jp}
the objective function is written down in term of canonical moments. Besides this, D-optimal designs for various models have been calculated in [2, 3, 4, 5, 6, 8, 9, 10, 11, 12, 13, 14, 20, 21, 24]. For example, D-optimal designs for weighted polynomial regression with a weight function \(x^\alpha(1-x)^\beta\) were found explicitly in [10] by using canonical moments. However, in most cases, an explicit form of the D-optimal design is unknown. We here consider polynomial regression models with some prior information. For example, D-optimal designs for this kind of models have been studied in [3, 8, 11]. D-optimal designs for polynomial regression models with only odd (or even) degree terms are calculated in [3]. Polynomial regression without intercept is considered in [11]. Polynomial regression models through origin is considered in [8].

On the other hand, the term integrable systems is used for nonlinear dynamical systems whose solutions can be written down concretely. For Hamiltonian systems with finite degree of freedom, their integrability is defined in the Liouville-Arnold theorem [1]. However, even now, there is no mathematical definition of integrability for nonlinear systems with infinite degree of freedom. This is why we call an explicitly solvable nonlinear system as an integrable system. Discrete integrable systems are discrete analogues of integrable systems. That is, it is well-known that integrable systems can be discretized such that discretized systems are also solvable.

Discrete integrable systems have been applied to numerical analysis. Typical examples are matrix eigenvalue algorithms [15, 22], and algorithms to compute matrix singular values [23].

An algorithm for calculating D-optimal designs for polynomial regression through a fixed point is proposed in [17]. In [17], the relationship between canonical moments and discrete integrable systems are used. In this thesis, we propose an algorithm for constructing D-optimal designs for polynomial regression with prior information, which is a generalized algorithm of [17], and the considered models include polynomial regression through origin [8], and some weighted polynomial regression as particular cases. Moreover the algorithm can be applied to some optimal designs, and it allows us to calculate a larger class of optimal designs. That means the relationship between canonical moments and discrete integrable systems expands the class of D-optimal designs which can be calculated.
2 A preliminary

This section gives a brief introduction of polynomial regression models, D-optimal designs, and canonical moments.

At first, we consider the following common linear regression model

\[ Y = \theta^T f(x) + \varepsilon, \]

\[ E[\varepsilon] = 0, \quad V[\varepsilon] = \sigma^2, \]

where \( f(x) = (f_0(x) \ f_1(x) \cdots f_{m-1}(x))^T \) denotes a known vector of linear independent functions, \( \theta = (\theta_0(x) \ \theta_1(x) \cdots \theta_{m-1}(x))^T \) denotes an unknown vector of parameters, \( \varepsilon \) denotes the error term. Here we assume each experiment has a statistically independent error term \( \varepsilon \).

Let \( \mathcal{P}_I \) be the set of probability measures on the borel set on \( I \). For given \( \mu \in \mathcal{P}_I \), let \( c_k \) denote the \( k \)th moment \( \int_I x^k d\mu(x) \). Suppose the number of experiments be \( n \), and experimental conditions \( x_1, x_2, \ldots, x_n \) should be in interval \([0,1]\). Here we consider design \( x_1, x_2, \ldots, x_n \) is corresponding to the probability measure \( \mu \in \mathcal{P}_{[0,1]} \) such that \( \mu(\{x\}) = \#\{k | x_k = x\} / n \). Then D-optimal designs are defined as probability measure \( \mu \in \mathcal{P}_{[0,1]} \) which maximizes the determinant of Fisher information matrix \( M_f(\mu) = \int_0^1 f(x) f(x)^T d\mu(x) \).

In the case of \((m-1)\)th polynomial regression, that is, in the case where \( f_k(x) = x^k \), the D-optimal design is defined as the optimization solution of the optimization problem

\[
\text{maximize } |c_{i+j}|_{i,j=0}^{m-1} \\
\text{subject to } \mu \in \mathcal{P}_{[0,1]}. \tag{1}
\]

Note that, in the optimization problem, while \( \mu(\{x\}) \) should be multiple of \( 1/n \) for all \( x \), we do not take a such constraint. Therefore we consider only the relaxation optimization problem. See [16] for details.

In the optimization problem \((1)\), the objective function is written down in terms of moments. However the constraint is complicated in terms of moments. To simplify the constraint, sometimes the optimization problem is rephrased in terms of canonical moments.

Now, we define canonical moments. Suppose we consider the set \( \mathcal{P}_{[0,1]} \) of the probability measures on \([0,1]\). For a given probability measure \( \mu \in \mathcal{P}_{[0,1]} \), let \( c_k^\mu \) denote the maximum of the \( k \)-th moment over the set of all measure
having moments $c_0, c_1, \ldots, c_{k-1}$. Similarly let $c_k^-$ denote the corresponding minimum. Canonical moments are defined by

$$p_k = \frac{c_k - c_{k-1}}{c_k^+ - c_k^-}, \quad k = 1, 2, \ldots, N,$$

(2)

where $N$ is the minimum of $j$ which satisfy $c_{j+1}^+ = c_{j+1}^-$. If $c_j^+ > c_j^-$ for an arbitrary positive integer $j$, let’s set $N = \infty$.

Canonical moments have the property that

$$\begin{align*}
&\left\{ p_k \in (0, 1), \quad k = 1, 2, \ldots, N - 1, \\
&\quad p_N \in \{0, 1\} \right. 
\end{align*}$$

(3)

Conversely, for a given arbitrary sequence $\{p_k\}_{k=1}^N$ which satisfies (3), there is a unique $\mu \in \mathcal{P}_{[0,1]}$ which has the canonical moments $\{p_k\}_{k=1}^N$.

It is to be noted that canonical moments have a Hankel determinant expression. Let $H_k^{(n)}, \overline{H}_k^{(n)}$ be the Hankel determinants defined by

$$
H_k^{(n)} = |c_{i+j+n}|_{i,j=0}^{k-1}, \quad \overline{H}_k^{(n)} = |c_{i+j+n} - c_{i+j+n+1}|_{i,j=0}^{k-1},
$$

(4)

where $k = 1, 2, \ldots, n = 0, 1, 2, \ldots$. We here set that $H_0^{(n)} = 1$, and that $H_k^{(n)} = 0$ if a matrix size $k$ is negative. The canonical moments $p_k$ have the following Hankel determinant expression:

$$p_{2k-1} = \frac{H_k^{(1)} \overline{H}_k^{(0)}}{H_k^{(0)} \overline{H}_k^{(1)}}, \quad p_{2k} = \frac{H_k^{(0)} \overline{H}_k^{(1)}}{H_k^{(1)} \overline{H}_k^{(0)}}, \quad k = 1, 2, \ldots.$$  

We introduce useful variable $\zeta_k$ by the transformation of canonical moments $p_k$

$$\begin{align*}
\zeta_0 &= 0, \quad \zeta_1 = p_1, \\
\zeta_k &= (1 - p_{k-1})p_k, \quad k = 2, 3, \ldots, N.
\end{align*}$$

(5)

Then $\zeta_k$ also have the Hankel determinant expression

$$\begin{align*}
\zeta_{2k-1} &= \frac{H_k^{(1)} H_k^{(0)}}{H_k^{(0)} H_k^{(1)}}, \quad \zeta_{2k} &= \frac{H_k^{(0)} H_k^{(1)}}{H_k^{(1)} H_k^{(0)}}, \quad k = 1, 2, \ldots.
\end{align*}$$
From this expression, Hankel determinants $H_m$ can be expressed in a product of $\zeta_k$ or of canonical moments $p_k$,

$$H_m^{(0)} = \prod_{k=1}^{m-1} (\zeta_{2k-1}\zeta_{2k})^{m-k}$$

$$= \left(\prod_{j=1}^{m-1} (1 - p_{2j})^{m-j-1}p_{2j}^{m-j}\right) \prod_{j=1}^{m-1} ((1 - p_{2j-1})p_{2j-1})^{m-j},$$

where $2m - 2 \leq N$. D-optimal designs for polynomial regression are calculated in [18] through the expression (6). Similar approaches for other D-optimal designs are described in the book [7].

3 An algorithm for calculating D-optimal designs for polynomial regression with prior information

In this section, we consider polynomial regression with prior information. In Subsection 3.2, polynomial regression with prior information is defined and formulated as a linear regression. Then we proposed an algorithm for calculating the D-optimal design for polynomial regression with prior information.

3.1 Generalized canonical moments and the nonautonomous discrete time Toda equation

At first, we generalize ordinary moments. For given moments $\{c_k\}_{k=0}^{\infty}$, let $c_k^{(T)}$ be defined by

$$c_k^{(T)} = c_{k+1} - \lambda c_k^{(T)}, \quad c_k^{(\phi)} = c_k,$$

where $T$ denotes a multiset. And let $H_k^{(T)}$ be its Hankel determinant $|c_{i+j}^{(T)}|_{i,j=0}^{k-1}$. Then canonical moments $p_k$ and variables $\zeta_k$ are expressed as

$$p_{2k} = -\frac{H_{k+1}^{(\phi)}H_k^{(0, -1)}}{H_k^{(0)}H_k^{(1, -1)}}, \quad p_{2k+1} = -\frac{H_{k+1}^{(0)}H_k^{(0, -1)}}{H_k^{(0)}H_k^{(1, -1)}}$$

$$\zeta_{2k} = \frac{H_{k+1}^{(\phi)}H_k^{(0, -1)}}{H_k^{(0)}H_k^{(\phi)}}, \quad \zeta_{2k+1} = \frac{H_{k+1}^{(0)}H_k^{(\phi)}}{H_k^{(0)}H_k^{(\phi)}}.$$

(7)
We define generalized canonical moments \( p_k^{(T)} \) and variable \( \zeta_k^{(T)} \) by
\[
P_{2k}^{(T)} = -\frac{H_{k+1}^{(T\{0\})} H_{k-1}^{(T\{0,1\})}}{H_k^{(T\{0\})} H_k^{(T\{-1\})}}, \quad P_{2k+1}^{(T)} = -\frac{H_{k+1}^{(T\{0\})} H_k^{(T\{0,-1\})}}{H_{k+1}^{(T\{0\})} H_k^{(T\{-1\})}},
\]
\[
\zeta_{2k}^{(T,s)} = \frac{H_{k+1}^{(T\{s\})} H_{k-1}^{(T\{s\})}}{H_k^{(T\{s\})} H_k^{(T)}}, \quad \zeta_{2k+1}^{(T,s)} = \frac{H_{k+1}^{(T\{s\})} H_k^{(T)}}{H_{k+1}^{(T\{s\})} H_k^{(T)}}, \quad \zeta_0^{(T)} = 0, \quad \zeta_1^{(T)} = P_1^{(T)}, \quad \zeta_k^{(T,0)} = (1 - P_{k-1}^{(T)}) P_k^{(T)}, \quad k = 2, 3, \ldots, N. \tag{9}
\]

Additionally variables \( \zeta_k^{(T)} \) is a determinant solution of nonautonomous discrete time Toda equation, namely, \( \zeta_k^{(T)} \) is satisfy nonautonomous discrete time Toda equation
\[
\zeta_{2k}^{(T\{\lambda_1, \lambda_2\})} + \zeta_{2k+1}^{(T\{\lambda_1\})} + \lambda_2 = \zeta_{2k+1}^{(T, \lambda_1)} + \zeta_{2k+2}^{(T, \lambda_1)} + \lambda_1, \quad \zeta_{2k+1}^{(T\{\lambda_1, \lambda_2\})} + \zeta_{2k+2}^{(T\{\lambda_1, \lambda_2\})} = \zeta_{2k+1}^{(T, \lambda_1)} \cdot \zeta_{2k+2}^{(T, \lambda_1)} \cdot. \tag{10}
\]

From (10), we obtain the following formula
\[
\zeta_{2k}^{(T, \lambda_1)} + \zeta_{2k+1}^{(T, \lambda_1)} + \lambda_2 = \zeta_{2k+1}^{(T, \lambda_2)} + \zeta_{2k+2}^{(T, \lambda_2)} + \lambda_1, \quad \zeta_{2k+1}^{(T, \lambda_1)} \cdot \zeta_{2k+2}^{(T, \lambda_2)} = \zeta_{2k+2}^{(T, \lambda_2)} \cdot. \tag{11}
\]

### 3.2 D-optimal designs for polynomial regression with prior information

We consider the \((m + S - 1)\)-th degree of polynomial regression
\[
Y = \sum_{k=0}^{m+S-1} \theta_k x^k + \varepsilon, \tag{12}
\]
where
\[
E[\varepsilon] = 0, \quad V[\varepsilon] = \sigma^2
\]
with the \(S = \sum_{j=1}^{l} b_j \) values as prior information
\[
\frac{d^k}{dx^k} g(x) \bigg|_{x=\beta_j}, \quad 0 \leq j < l, \quad 0 \leq k < b_j, \tag{13}
\]
where \( g(x) = E[Y|x] = \sum_{k=0}^{m+S-1} \theta_k x^k \), \( b_0, b_1, \ldots, b_{l-1} \) are positive integers, and \( \beta_0, \beta_1, \ldots, \beta_{l-1} \) are arbitrary distinct real values. That means we consider the cases where the exact \( S \) values (13) are known before experiments. Note that \( \beta_k \) do not have to be in \( \mathcal{X} = [0,1] \). We call the model (12) \( \text{PRM}_m(\beta, b) \), for short, where \( \beta = (\beta_0, \beta_1, \ldots, \beta_{l-1}), b = (b_0, b_1, \ldots, b_{l-1}) \).

There are multiple ways to consider the model \( \text{PRM}_m(\beta, b) \) as linear regression models. However the D-optimal design for the model \( \text{PRM}_m(\beta, b) \) is defined uniquely, since D-optimal designs for linear regression models depend on a linear space spanned by bases functions only (see [7, Theorem 5.5.1]). The D-optimal designs are formulated as the following theorem. A proof of the theorem is given in Appendix.

**Theorem 3.1.** The D-optimal design for polynomial regression with prior information \( \text{PRM}_m(\beta, b) \) is defined as the optimal solution of the optimization problem

\[
\text{maximize } H_m^{(T)} \quad \text{subject to } \mu \in \mathcal{P}_{[0,1]}.
\]

where the multiset \( T \) satisfies the number of \( \beta_k \) in the \( T \) is \( 2b_k \), that is, let \( m_T(x) \) be the multiplicity function, then

\[
m_T(x) = \begin{cases} 
2b_k & (x = \beta_k) \\
0 & \text{(otherwise)}
\end{cases}.
\]

Note that the D-optimal design for \( \text{PRM}_m(\beta, b) \) is equivalent to the D-optimal design for weighted polynomial regression model

\[
Y = \sum_{k=0}^{m-1} \theta_k x^k + \varepsilon,
\]

\[
E[\varepsilon] = 0, \quad V[\varepsilon] = \frac{\sigma^2}{w(x)}, \quad w(x) = \prod_{k=0}^{l-1} (x - \beta_k)^{2b_k}.
\]

Here we propose an algorithm for rephrasing the optimization problem (14) in terms of canonical moments. In the algorithm, the two formulas (16), (17) and the nonautonomous discrete time Toda equation (10) are used.

At first, we describe the objective function \( H_m^{(T)} \) by using the value \( c_k^{(T,s)} \) corresponding to generalized canonical moments. We obtain the formula
which is similar to (6)

\[ H_m^{(T)} = \left( c_0^{(T)} \right)^m \prod_{j=1}^{m-1} \left( \zeta_j^{(T,0)} \zeta_j^{(T,0)} \right)^{m-j}. \] (16)

Then we describe the objective function \( H_m^{(T)} \) in terms of the value \( \zeta_k^{(\phi,0)} \) corresponding to canonical moments. Here by using the nonautonomous discrete time Toda equation (10) and the formula (11), \( \zeta_k^{(T,s)} \) can be expressed in terms of \( \zeta_1^{(\phi,0)}, \zeta_2^{(\phi,0)}, \ldots \). And we obtain the formula about \( c_0^{(T)} \)

\[ \zeta_1^{(T,s)} = \frac{c_0^{(T \cup \{s\})}}{c_0^{(T)}}, \quad c_0^{(\phi)} = 1, \] (17)

then \( c_0^{(T)} \) also can be expressed in terms of \( \zeta_1^{(\phi,0)}, \zeta_2^{(\phi,0)}, \ldots \) by using the formula.

Lastly we describe the objective function \( H_m^{(T)} \) in terms of canonical moments by using the relationship (5).

By putting it all together, the proposed algorithm for calculating the D-optimal design for polynomial regression with prior information (12) is described as follows.

| The algorithm for calculating D-optimal designs for PRM_m(\beta, b) |
|---------------------------------------------------------------|
| Step 1. By using the formula (16), describe the objective function \( H_m^{(T)} \) in terms of \( \zeta_k^{(T,s)} \) and \( c_0^{(T)} \). |
| Step 2. By using the nonautonomous discrete time Toda equation (10) and the formulas (11), (17), describe the objective function \( H_m^{(T)} \) in terms of \( \zeta_k^{(\phi,0)} = \zeta_k \). |
| Step 3. By using the relationship (5), describe the objective function \( H_m^{(T)} \) in terms of canonical moments \( p_k \). |
| Step 4. Find canonical moments which maximize the objective function \( H_m^{(T)} \). |

4 Application of the algorithm for calculating some D-optimal designs

In this section, we introduce two examples of application of our algorithm. In Subsection 4.1 robust D-optimal designs for approximate polynomial
regression with prior information is considered. This model is generalized model considered by [10]. In Subsection 4.2 maximin optimal designs for estimating a function of parameters on weighted polynomial regression. We consider the generalized case of the case considered by [6].

4.1 Robust D-optimal designs for approximate polynomial regression with prior information

In this subsection, let the design space be \( \mathcal{X} = [-1, 1] \) instead of \([0, 1]\). There is one to one correspondence between \( \mu \in \mathcal{P}_{[0, 1]} \) and a symmetric measure \( \xi \in \mathcal{P}_{[-1, 1]} \) such that

\[
\mu([0, x^2]) = \xi([-x, x]).
\]

The approximate polynomial regression model is described as

\[
Y = \sum_{k=0}^{m-1} \theta_k x^k + x^m \psi(x) + \varepsilon,
\]

where \( \psi \) denotes an unknown function. Let the best linear unbiased estimator be \( \hat{\theta}(\psi) \) when we estimate as \( \psi(x) \) is considered as 0. Then we obtain

\[
E[\hat{\theta}(\psi) - \hat{\theta}(0)] = B_m^{(\phi)}(\xi)r(\phi)
\]

\[
V[\hat{\theta}(\psi)] = (\sigma^2/n)B_m^{(\phi)}(\xi)
\]

where \( \xi \) is a design, \( n \) is the number of observations, and

\[
r(\psi) = \int_{-1}^{1}(1, x, \ldots, x^{m-1})^T x^m \psi(x) d\xi(x),
\]

\[
B_m^{(\phi)} = (c_{i+j}(\xi))_{i,j=0}^{m-1}.
\]

For given a continuous function \( \eta(x) \) and a positive number \( d \), maximin optimal design is defined as

\[
\text{maximize } H_m^{(\phi)}(\xi)
\]

subject to \( \xi \in \mathcal{P}_{[-1, 1]}, \quad \sup_{|\psi| \leq |\eta|} r(\psi)^T(B_m^{(\phi)})^{-1} r(\psi) \leq d. \)
In [10], the case where
\[ \eta(x) = |x|^\alpha, \quad \alpha \in \mathbb{Z}_{\geq 0} \]  
(18)
is considered, and it is shown that the constraint \( \sup_{|\psi| \leq |\eta|} r(\psi)^T (B_m^{(\phi)})^{-1} r(\psi) \leq d \) is described in terms of canonical moments as
\[
\sup_{|\psi| \leq |\eta|} r(\psi)^T (B_m^{(\phi)})^{-1} r(\psi) = \sum_{i=\lfloor\alpha/2\rfloor+1}^{\lfloor(m+\alpha)/2\rfloor} S_{i,m+\alpha-i}(\mu)^2 \prod_{j=1}^{m+\alpha-2i} \zeta_j(\mu), 
\]  
(19)
where \( S_{i,j}(\mu) \) is defined recursively as
\[
S_{i,j}(\mu) = \begin{cases} 
0, & 0 \leq j < i, \\
1, & i = 0, \ j > 0, \\
S_{i,j-1}(\mu) + \zeta_{j-i+1}(\mu)S_{i-1,j}(\mu), & 0 < i \leq j.
\end{cases}
\]

Now we consider the approximate polynomial regression model with prior information, namely,
\[
Y = \sum_{k=0}^{2S+m-1} \theta_k x^k + x^{2S+m} \psi(x) + \varepsilon, 
\]  
(20)
with the \( 2S \) values as prior information
\[
\frac{d^k}{dx^k} g(x) \bigg|_{x=\beta_j}, \\
\frac{d^k}{dx^k} g(x) \bigg|_{x=-\beta_j}, \quad 0 \leq j < l, \quad 0 \leq k < b_j, 
\]  
(21)
where \( g(x) = E[Y|x] = \sum_{k=0}^{m+S-1} \theta_k x^k \), and \( \beta_0, \beta_1, \ldots, \beta_{l-1} \) are arbitrary distinct real values. Note that prior information (21) must be symmetric with respect to the origin.

We can show that the optimization problem corresponding to the model (20) is the following by similar calculation to [10]
\[
\text{maximize } H_m^{(T')} (\xi) \\
\text{subject to } \xi \in \mathcal{P}_{[-1,1]}, \quad \sup_{|\psi| \leq |\eta|} r^{(T')} (\psi)^T (B_m^{(T')})^{-1} r^{(T')} (\psi) \leq d,
\]  
(22)
where \( T' \) denotes the multiset satisfying

\[
m_{T'}(x) = \begin{cases} 
2b_k & (x = \beta_k) \\
2b_k & (x = -\beta_k) \\
0 & \text{(otherwise)}
\end{cases}
\]

and

\[
B_{m}^{(T')}(\xi) = (c^{(T')}_{i,j})_{i,j=0}^{m-1}
\]

\[
r^{(T')}(\psi) = \int_{-1}^{1} (1, x, \ldots, x^{m-1})^T x^m \psi(x) \left( \prod_{j=0}^{l-1} (x - \beta_j)(x + \beta_j) \right) d\xi(x).
\]

The constraint of (22) corresponding to (19) is described in terms of generalized canonical moments as

\[
(c_0^{(T')})(\xi)^{-1} \sum_{i=[\alpha/2]+1}^{[(m+\alpha)/2]} S_{i,m+\alpha-i}(\mu)^2 \prod_{j=1}^{m+\alpha-2i} \zeta_j^{(T,0)}(\mu),
\]

where \( T \) is the same as (15), and

\[
S_{i,j}^{(T)}(\mu) = 0, \quad 0 \leq j < i,
\]

\[
S_{i,j}^{(T)}(\mu) = 1, \quad i = 0, \quad j > 0,
\]

\[
S_{i,j}^{(T)}(\mu) = S_{i,j-1}^{(T)}(\mu) + \zeta_j^{(T,0)}(\mu) S_{i-1,j}^{(T)}(\mu), \quad 0 < i \leq j.
\]

Hence we can obtain the expression of the optimization problem corresponding to (20) in terms of canonical moments by using our algorithm.

### 4.2 Maximin optimal designs for estimating a function of parameters on weighted polynomial regression

Consider the weighted polynomial regression

\[
Y = \sum_{k=0}^{m-1} \theta_k x^k + \varepsilon,
\]

\[
E[\varepsilon] = 0, \quad V[\varepsilon] = \sigma^2 w(x), \quad w(x) = \prod_{k=0}^{l-1} (x - \beta_k)^{2b_k}.
\]
In this subsection, we consider an optimal design for estimating \( g_{m-1}(\theta_{m-1}) + g_{m-2}(\theta_{m-2}) + \cdots + g_0(\theta_0) \), where \( g_k \) is a polynomial. In this case, the inverse of the asymptotic variance of the estimator is

\[
\gamma(\mu, \theta) = \sum_{k=0}^{m-1} \left( \frac{d}{d\theta_k} g_k(\theta_k) \right)^2 \psi_k^{(1)}(\mu),
\]

where \( \psi_k^{(1)}(\mu) = H_{k+1}^{(T)}/H_{k}^{(T)} \), and \( T \) is the same as \([15]\). Since the variance of estimator depends on the unknown parameters \( \theta_k \), we consider maximin optimal design defined as the optimization solution of the optimization problem

\[
\begin{align*}
\text{maximize} & \quad \min_{\theta \in \Theta} \gamma(\mu, \theta) \\
\text{subject to} & \quad \mu \in P_{[0,1]}
\end{align*}
\]

where \( \Theta \) is a given parameter space. Suppose the parameter space \( \Theta = \{\theta \mid s_k \leq \theta_k \leq t_k\} \).

From [6, Theorem 3.1], the optimal solution of the optimization problem

\[
\begin{align*}
\text{maximize} & \quad \int_{\Theta} \gamma(\mu, \theta)^p d\pi(\theta) \\
\text{subject to} & \quad \mu \in P_{[0,1]},
\end{align*}
\]

(23)

converges weakly to the maximin optimal design as \( p \to -\infty \), where

\[
d\pi(\theta) = d\theta \prod_{k=0}^{m-1} h_k(\theta_k),
\]

\[
h_k(\theta_k) = \begin{cases} 
\frac{d}{d\theta_k} \left( \frac{d}{d\theta_k} g_k(\theta_k) \right)^2 & (\text{deg } g_k \geq 2) \\
1 & (\text{otherwise})
\end{cases}
\]

Then we can calculate the integral in the objective function of the (23). And we can express \( \psi_k^{(1)}(\mu) \) in terms of canonical moments by our algorithm. Therefore, after expressing the optimization problem (23) in terms of canonical moments, we can obtain an approximate maximin optimal design by solving (23) numerically for small \( p \).
A The proof of Theorem 3.1

It can be turn out that the optimization problem (14) corresponding to \( \text{PRM}_m(\beta, b) \) corresponds to the vector of basis functions

\[
f(x) = \left( \prod_{j=0}^{l-1} (x - \beta_j)^{b_j} \right) (1, x, \ldots, x^{m-1})^T. \tag{24}
\]

Let \( g_k(x) = (1, x, \ldots, x^{k-1}) \) be the vector of basis functions for polynomial regression, then the vector (24) of basis functions corresponding to \( \text{PRM}_m((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0, b_1, \ldots, b_{l-1})) \) is expressed as

\[
f(x) = \prod_{j=0}^{l-1} (x - \beta_j)^{b_j} g_m(x). \tag{25}
\]

To prove Theorem 3.1 it suffices to show that \( \text{PRM}_m((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0, b_1, \ldots, b_{l-1})) \) corresponds to the vector of basis functions. Let us prove it by the principle of induction. By the symmetricity of \( \beta_j \) and \( b_j \), we can assume that \( \text{PRM}_{m+1}((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0, b_1 - 1, \ldots, b_{l-1})) \) corresponds to the vector of basis functions

\[
f(x) = (x - \beta_0)^{b_0-1} \left( \prod_{j=1}^{l-1} (x - \beta_j)^{b_j} \right) g_{m+1}(x).
\]

Let \( M(x) = \prod_{j=1}^{l-1} (x - \beta_j)^{b_j} \), then the linear regression model \( \text{PRM}_{m+1}((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0 - 1, b_1, \ldots, b_{l-1})) \) is described as

\[
Y = (x - \beta_0)^{b_0-1} M(x) \sum_{k=0}^{m} \theta_k x^k + \varepsilon.
\]

Thus the linear regression model \( \text{PRM}_m((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0, b_1, \ldots, b_{l-1})) \) is described as

\[
Y = (x - \beta_0)^{b_0-1} M(x) \sum_{k=0}^{m} \theta_k x^k + \varepsilon. \tag{26}
\]

with one given value as prior information

\[
\frac{d^{b_0-1}}{dx^{b_0-1}} \left( (x - \beta_0)^{b_0-1} M(x) \sum_{k=0}^{m} \theta_k x^k \right) \bigg|_{x = \beta_0}.
\tag{27}
\]
Since
\[
\frac{d^k}{dx^k}(x - \beta_0)^{b_0 - 1} = 0, \quad k = 0, 1, \ldots, b_0 - 2,
\]
the value (27) becomes
\[
(b_0 - 1)!M(\beta_0)\sum_{k=0}^{m} \theta_k \beta_0^k
\]
by the general Leibniz rule. Hence we obtain the value
\[
\alpha = \sum_{k=0}^{m} \theta_k \beta_0^k
\]
from prior information (27).

From (28), substitute \(\theta_0 = \alpha - \sum_{k=1}^{m} \theta_k \beta_0^k\) into the model (26), we obtain
\[
Y = (x - \beta_0)^{b_0 - 1} M(x) \left( \sum_{k=1}^{m} \theta_k x^k - \sum_{k=1}^{m} \theta_k \beta_0^k + \alpha \right) + \varepsilon. \tag{29}\]

When we obtain a response \(y_k\) by observation at the experimental condition \(x_k\), we can calculate the value \(y_k - (x_k - \beta_0)^{b_0 - 1} M(x_k) \alpha\) easily. Thus we can ignore the term \((x - \beta_0)^{b_0 - 1} M(x) \alpha\) from the model (29), then we obtain the model
\[
Y = (x - \beta_0)^{b_0 - 1} M(x) \sum_{k=1}^{m} \theta_k (x^k - \beta_0^k) + \varepsilon. \tag{30}\]

Here the vector of basis functions corresponding to the model (30) is
\[
f(x) = (x - \beta_0)^{b_0 - 1} M(x) \begin{pmatrix} x - \beta_0 \\ x^2 - \beta_0^2 \\ \vdots \\ x^m - \beta_0^m \end{pmatrix}. \tag{31}\]

Let the non-singular matrix \(A\) be
\[
A = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ -\beta_0 & 1 & 0 & \cdots & 0 \\ 0 & -\beta_0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}
\]

14
then, by multiplying $A$ to the vector $\mathbf{31}$ of basis functions from left,

$$Af(x) = (x - \beta_0)^{b_0 - 1}M(x) \begin{pmatrix} x - \beta_0 \\ x^2 - \beta_0^2 - \beta_0(x - \beta_0) \\ \vdots \\ x^m - \beta_0^m - \beta_0(x^{m-1} - \beta_0^{m-1}) \end{pmatrix}$$

$$= (x - \beta_0)^{b_0 - 1}M(x) \begin{pmatrix} x - \beta_0 \\ x(x - \beta_0) \\ \vdots \\ x^{m-1}(x - \beta_0) \end{pmatrix}$$

$$= (x - \beta_0)^{b_0}M(x)g_m(x).$$

Thus we obtain (25).

References

[1] Arnold, V. I.: *Mathematical Methods of Classical Mechanics*, Springer-Verlag, New York-Heidelberg, 1978.

[2] Biedermann, S., Dette, H. and Hoffmann, P.: Constrained optimal discrimination designs for Fourier regression models, *Ann. Inst. Stat. Math.*, 61 (2009), 143–157.

[3] Dette, H.: Optimal designs for a class of polynomial regression of odd or even degree, *Ann. Stat.*, 20 (1992), 238–259.

[4] Dette, H. and Franke, T.: Constrained $D$- and $D_1$-optimal designs for polynomial regression, *Ann. Stat.*, 28 (2000), 1702–1727.

[5] Dette, H. and Franke, T.: Robust designs for polynomial regression by maximizing a minimum of $D$- and $D_1$-efficiencies, *Ann. Stat.*, 29 (2001), 1024–1049.

[6] Dette, H., Haines, L. M. and Imhof, L. A.: Maximin and Bayesian optimal designs for regression models, *Statistica Sinica*, 17 (2007), 463–480.
[7] Dette, H. and Studden, W.: *The Theory of Canonical Moments with Applications in Statistics, Probability and Analysis*, Wiley, New York, 1997.

[8] Fang, Z.: $D$-optimal designs for polynomial regression models through origin, *Stat. Prob. Lett.*, 57 (2002), 343–351.

[9] Fang, Z.: Some robust designs for polynomial regression models, *Can. J. Stat.*, 34 (2006), 623–638.

[10] Fang, Z. and Wiens, D. P.: Robust regression designs for approximate polynomial models, *J. Stat. Plann. Inference*, 117 (2003), 305–321.

[11] Huang, M. N. L., Chang, F. C. and Wong, W. K.: $D$-optimal designs for polynomial regression without intercept, *Statistica Sinica*, 5 (1995), 441–458.

[12] Lau, T. S.: $D$-optimal designs on the unit $q$-ball, *J. Stat. Plann. Inference*, 19 (1988), 299–315.

[13] Lau, T. S. and Studden, W. J.: Optimal designs for trigonometric and polynomial regression using canonical moments, *Ann. Stat.*, 13 (1985), 385–394.

[14] Lim, Y. B. and Studden, W. J.: Efficient $D_s$-optimal designs for multivariate polynomial regression on the $q$-cube, *Ann. Stat.*, 16 (1988), 1225–1240.

[15] Nakamura, Y.: A tau-function of the finite nonperiodic Toda lattice, *Phys. Lett. A.*, 195 (1988), 346–350.

[16] Pukelsheim, F.: *Optimal Design of Experiments*, Wiley, New York, 1993.

[17] Sekido, H.: An algorithm for calculating $D$-optimal designs for polynomial regression through a fixed point, *J. Stat. Plann. Inference*, 142 (2012), 935–943.

[18] Studden, W. J.: $D_s$-optimal designs for polynomial regression using continued fractions, *Ann. Stat.*, 8 (1980), 1132–1141.
[19] Studden, W. J.: Optimal designs for weighted polynomial regression using canonical moments, *Statistical Decision Theory and Related Topics III*, 2 (1982), 335–350.

[20] Studden, W. J.: Some robust-type $D$-optimal design in polynomial regression, *J. Amer. Stat. Assoc.*, 77 (1982), 916–921.

[21] Studden, W. J.: Note on some $\Phi_p$ optimal design for polynomial regression, *Ann. Stat.*, 17 (1989), 618–623.

[22] Symes, W. W.: The $QR$ algorithm and scattering for the finite nonperiodic Toda lattice, *Physica D.*, 4 (1982), 275–280.

[23] Tsujimoto, S., Nakamura, Y. and Iwasaki, M.: The discrete Lotka-Volterra system computes singular values, *Inverse Problems*, 17 (2001), 53–58.

[24] Zen, M. M. and Tsai, M. H.: Criterion-robust optimal designs for model discrimination and parameter estimation in Fourier regression models, *J. Stat. Plann. Inference*, 124 (2004), 475–487.