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D – optimal Design in Polynomial Spline Regression†

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ABSTRACT

For the polynomial spline regression with fixed knots, some properties of the D−optimal design are discussed. Also the D−optimal design for some cases are found analytically by using a normalized B−spline basis for $S(\mathcal{P}_m : \mathrm{k} : \Delta)$. Based on the Kiefer−Wolfowitz equivalence theorem, the D−optimal design for some cases are found by numerical methods.

1. Introduction

The present paper is concerned with D−optimal designs in the polynomial spline regression with fixed knots.

We consider the interval [a, b] and choose h fixed knots, $s_1, \cdots, s_h$ such that $a=s_0<s_1<\cdots<s_h<s_{h+1}=b$. Let $\Delta=\{s_i\}_0^h$ be a partition of [a, b] into h+1 subintevals $I_i=[s_i, s_{i+1})$, i=0, ⋯, h. Let m be a positive integer and $\mathbf{k}'=(k_1, \cdots k_h)$ be a vector of integers with $1\le k_i\le m-1$, $i=1, \cdots, h$. We define

$$\mathcal{P}_m = \{p(x)=\sum^{m} a_i x^{i-1},\ a_1, \cdots a_m,\ x \text{ real}\}$$

and call it the space of polynomials of order m.

Definition 1. *We call the space*

$S(\mathcal{P}_m : \mathbf{k} : \Delta)=\{s :$ *there exist polynomials* $p_0, \cdots, p_h$ in $\mathcal{P}_m$ *such that*
$s(x)=p_i(x)$ *for* $x\in I_i$, $i=0, \cdots h$ *and* $D^j p_{i-1}(s_i)=D^j p_i(s_i)$
for $j=0, 1, \cdots, m-1-k_i$, $i=1, \cdots, h\}$

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the space of polynomial splines of order m with knots $s_1, \cdots, s_h$ *of multiplicities* $k_1, \cdots, k_h$. *Here* D^j *is the* $j-th$ *order derivative of polynomial* $p_i(x)$.

The function x_+^j is defined by

$$x_+^j = \begin{cases} x^j & \text{if } x \geq 0 \\ 0 & \text{o.w.} \end{cases}$$

Then a basis for $S(\mathcal{P}_m : \mathbf{k} : \Delta)$ is given by

$$1,\ x,\ \cdots,\ x^{m-1},\ (x-s_i)_+^{m-k_i}, \cdots,\ (x-s_i)_+^{m-1},\ 1 \leq k_i \leq m-1,\ 1 \leq i \leq h, \qquad (1)$$

which are our vector of regression functions. Studden(1971) and Park(1978) have some numerical results on the saturated D−optimal design. In section 2, some properties of the D−optimal design are discussed. Also the D−optimal design for some cases are found analytically by using a normalized B−spline basis for $S(\mathcal{P}_m : \mathbf{k} : \Delta)$. Based on the the Kiefer−Wolfowitz equivalence theoem, the D−optimal design for some cases are found by numerical methods in section 3.

2. D−optimal Design

A design ξ is a probability measure on the interval $[a, b]$. The information matrix is given by

$$M(\xi) = \int f(x) f(x)' \xi(dx).$$

A design ξ^* is D−optimal iff $|M(\xi^*)| = Max_\xi |M(\xi)|$. The D−optimality criterion is known by the celebrated Kiefer−Wolfowitz theorem to be equivalent to the G−optimality criterion. So the design ξ^* is D−optimal iff the variance function $d(x, \xi^*) \leq m+K$ for any x, where $d(x, \xi^*) = f(x)' M^{-1}(\xi^*) f(x)$ and $K = \Sigma^h_{i=1} k_i$, i.e., $m+K$ is the number of parameters in the model.

W.L.O.G., assume that x is transformed linearly so that $-1 \leq x \leq 1$ since the D−optimality criterion is invariant under nonsingular transformation of $f(x)$. Suppose that ξ_u is the D−optimal design for $S(\mathcal{P}_m : \mathbf{k} : \Delta)$.

Lemma 1. *-1 and 1 are in the support of the D−optimal design* ξ_u.

Proof. We take $f(x)$ as a basis given in (1). Accoridng to the Binet−Cauchy formula, $|M(\xi)|$ can be expressed as a linear combination of

$$|\, \| f_i(x_{l_j}) \|^{m+K}_{i,j=1} |^2,$$

where $\{x_{l_1}, \cdots, x_{l_{m+K}}\} \subset Supp(\xi)$, the support of a design ξ. So it suffies to show that $|\, \| f_i(x_j) \|^{m+K}_{i,j=1} |$ is a decreasing function of x_1 or increasing function of x_{m+K} while all the other x_i's are fixed.

Define F(t) by

$$F(t)=M\begin{pmatrix} x_1 & \cdots & x_{m+K-1} & t \\ f_1(x) & \cdots & f_{m+K-1}(x) & f_{m+K}(x) \end{pmatrix}. \tag{2}$$

Then it can be easily checked that $|F(t)|$ had m+K−1 zeros at x_i, $i=1, \cdots, m+K-1$. It follows from the Rolle's theorem that $\frac{d}{dt}|F(t)|$ has m+K−2 zeros and each of those is in (x_i, x_{i+1}), $i=1, \cdots, m+K-1$. So $\frac{d}{dt}|F(t)|$ is positive on $(x_{m+K-1}, 1]$(Theorem 4.64, Schumaker(1981)) and then, $|F(t)|$ is increasing. Similarly $|F(t)|$ is a decreasing function while $x_2, \cdots, x_{m+K}$ being fixed. □

The following lemma shows that the D−optimal design has the symmetric property with respect to knots.

Lemma 2. *Suppose* ξ_u *is the D−optimal design for* $S(\mathcal{P}_m : \mathbf{k} : \Delta)$. *Define* $\xi_{-u}(x)=\xi_u(-x)$. *Then* ξ_{-u} *is the D−optimal design for* $S(\mathcal{P}_m : \mathbf{k}' : \Delta')$, *where* $k_i'=k_{h-i+1}$ *and* $s_i'=-s_{h-i+1}$.

Proof. Define g(x)=−x and ξ_g by $\xi_g(x)=\xi(-x)$. Take $f(x)$, $f_g(x)$ as a basis of $S(\mathcal{P}_m : \mathbf{k} \mid \Delta)$, $S(\mathcal{P}_m \mid \mathbf{k}' : \Delta')$ given in (1), respectively. Note that

$$\begin{aligned}(-x-s_i)^l_+ &= (x+s_i)^l_- \\ &= -(x+s_i)^k+(x+s_i)^l_+ \\ &= -\sum_{j=0}^{l}\binom{l}{j}(s_i)^{l-j}x^j+(x+s_i)^l_+.\end{aligned}$$

Then, simple algebra shows that $f(gx)=H_L f_g(x)$, where H_L is the lower triangular matrix whose absolute values of diagonal elements are all equal to 1. Thus,

$$\begin{aligned}\left|\int f(x)f(x)'\xi_g(dx)\right| &= \left|\int f(gx)f(gx)'\xi(dx)\right| \\ &= |H_L|^2 \cdot |f_g(x)f_g(x)'\xi(dx)| \\ &= \left|\int f_g(x)f_g(x)'\xi(dx)\right|.\end{aligned}$$

So the lemma follows. □

For both ease of evaluation and a well−conditioned design matrix, it is desired to construct a basis for $S(\mathcal{P}_m : \mathbf{k} : \Delta)$ consisting of splines with relatively small supports. We shall use the normalized B−splines basis from now on. For the definitions and related properties of B−splines, refer to Schumaker(1981).

Next, we consider $S(\mathcal{P}_m : \mathbf{k} : \Delta)$ with $k_i=m-1$, $i=1, \cdots, h$.

Theorem 1. *Suppose* $k_i=m-1$, $i=1, \cdots, h$. *Then the D−optimal design* ξ_u *has uniform mass* $1/(m+K)$ *over*

$$\{-1, x^\circ_{01}, \cdots, x^\circ_{0(m-2)}, s_1, x^\circ_{11}, \cdots, s_h, x^\circ_{h1}, \cdots, x^\circ_{h(m-2)}, 1\},$$

where

$$x^{\circ}_{ij}=\frac{s_{i+1}-s_i}{2}(1+x_j^*)+s_i,\ i=0,\cdots,h,\ j=1,\cdots,m-2 \quad (3)$$

and x_j^*'*s are zeros of the derivative of the* $(m-1)$*-th degree Legendre polynomial.*

Proof. It follows from Studden & Van Arman's theorem(Studden & Van Arman(1969)) that the D-optimal design is saturated and $Supp(\xi_u)$ has all the s_i's and m-2 points in (s_i, s_{i+1}), $i=0,\cdots,h$. Since $k_i=m-1$ for any i, we get $B_{m+l(m-1)}(s_l)=1$, $l=0,\cdots,h$ from Theorem 4.9 in Schumaker(1981). Suppose ξ is a admissible and has uniform mass over $\{x_1,\cdots,x_{m+K}\}$. Recalling that $\Sigma_1^{m+K} B_i(x)=1$ and $B_i(x)\geq 0$, we get

$$|M_B^{m,u}(\xi)| = \left(\frac{1}{m+K}\right)^{m+K} \left| \ \| B_i^m(x_j) \|_{i,j=1}^{m+K} \right|^2$$

$$=\left(\frac{1}{m+K}\right)^{m+K} \prod_{l=0}^{h} \left| \ \|B_i^m(x_j)\|_{i,j=2+l(m-1)}^{2+l(m-1)+(m-3)} \right|^2,$$

in which $\left| \ \|B_j^m(x_i)\|_{i,j=2+l(m-1)}^{2+l(m-1)+(m-3)} \right|^2$ is proportional to the determinant of the information matrix of ξ_l for the (m-1)-th degree polynomial regression on $[s_l, s_{l+1}]$, where ξ_l has uniforms mass over $\{s_l, x_{2+l(m-1)}, \cdots, x_{2+l(m-1)+(m-3)}, s_{l+1}\}$. Thus the theorem follows from the result in Hoel (1958). □

Park(1978) gives the D-optimal design among the class of saturated desings for quadratic regression with one simple knot by maximizing determinants of the information matrix numerically. The following theorem shows analytically that design is in fact D-optimal.

Theorem 2. *For quadratic splines with one simple knot, i.e., $m=2$, $h=1$ and $k_1=1$,* the D-optimal design ξ_u *has uniform mass over* $\{-1, x_2(x), x_3(s), 1\}$,

$$\textit{where } x_2(s)=\frac{-3s^2+6s+1}{8}-\frac{\sqrt{9s^5-9s^4-62s^3-10s^2+85s+51}}{8\sqrt{s+3}}$$

$$\textit{and} \qquad x_3(s)=-x_2(-s). \quad (4)$$

Proof. By Studden & Van Arman's thoerem, the support of any admisible design has at most one point in $(-1,s)$ or $(s,1)$. So it suffices to consider a class of designs which have the uniform mass over $\{-1, x_2, x_3, 1\}$, where $-1<x_2<s<x_3<1$. Thus, find $x_2(s)$ and $x_3(s)$ such that

$$D\begin{pmatrix} -1 & x_2 & x_3 & 1 \\ B_1^3(x) & B_2^3(x) & B_3^3(x) & B_4^3(x) \end{pmatrix}=B_2^3(x_2)B_3^3(x_3)-B_2^3(x_3)B_3^3(x_2) \quad (5)$$

is maximized. From the recurrence relation of the B-splines,

$$B_2^3(x_2)=\frac{(x_2+1)(s-x_2)}{(1+s)^2}+\frac{(1-x_2)(x_2+1)}{2(1+s)},\quad B_2^3(x_3)=\frac{(1-x_3)^2}{2(1-s)},$$

$$B_3^3(x_2)=\frac{(x_2+1)^2}{1(1+s)} \text{ and } B_3^3(x_3)=\frac{(1-x_3)(1+x_3)}{2(1-s)}+\frac{(1-x_3)(x_3-s)}{(1-s)^2}. \tag{6}$$

Substituting (5) into (4), we get

$$D\begin{pmatrix} -1 & x_2 & x_3 & 1 \\ B_1^3(x) & B_2^3(x) & B_3^3(x) & B_4^3(x) \end{pmatrix}$$

$$=\frac{(1+x_2)(1-x_3)(-2s^2+(s^2+2s-1)x_2-(s^2-2s-1)x_3-2x_2x_3)}{(1+s)^2(1-s)}. \tag{7}$$

Simple algebra shows that (6) is maximized at

$$x_2(s)=\frac{-3s^2+6s+1}{8}-\frac{\sqrt{9s^5-9s^4-62s^3-10s^2+85s+51}}{8\sqrt{s+3}}$$

$$\text{and} \qquad x_3(s)=-x_2(-s). \tag{8}$$

Thus the D-optimal design ξ_u has uniform mass over $\{-1, x_2(s), x_3(s), 1\}$. □

3. Numerical Results

For the cubic, 4th, 5th degree polynomial spline regression with one and two simple knots, the determinant $| \, \|B_i^m(x_j)\|_{i,j=1}^{m+K} |$ was maximized on the VAX 11/780 over $-1=x_1<x_2<\cdots<x_{m+K}=1$ to get the D-optimal design, say ξ_u^*, among saturated designs. Table 1 and 2 list support points $x_i(s)$, $2\leq i\leq m+K-1$, in $(0,1)$ of ξ_u. The variance function $d(x,\xi_u^*)$ was computed numerically and found to be $\leq m+K$ to five decimal places with maxima occurring at points in the support of ξ_u^*. Thus the equivalence theorem by Kiefer & Wolfowitz(1961) implies that ξ_u^* is the D-optimal design in a numerical sense. Like the case of quadratic splines with one simple knot, it is interesting to check that $x_i(s)$, $2\leq i\leq m$, is increasing as the knot value s is increased.

Table 1. Interior Support of the D−optimal Design with one Simple Knot

	s	.0	.2	.4	.6	.8
m=4	x_2	−.6287	−.5843	−.5470	−.5145	−.4806
	x_3	.0	.1036	.1928	.2732	.3599
	x_4	.6287	.6785	.7330	.7964	.8863
m=5	x_2	−.7521	−.7276	−.7061	−.6878	−.6722
	x_3	−.2704	−.2061	−.1470	−.0954	−.0509
	x_4	.2704	.3420	.4224	.5004	.5711
	x_5	.7521	.7808	.8156	.8573	.9104
m=6	x_2	−.8232	−.8078	−.7949	−.7839	−.7747
	x_3	−.4567	−.4129	−.3573	−.3423	−.3146
	x_4	.0	.0658	.1269	.1836	.2326
	x_5	.4567	.5071	.5648	.6303	.6936
	x_6	.8232	.8418	.8646	.8935	.9317

Table 2. Interior Support of the D−optimal Design with Two Simple Knots

	(s_1, s_2)	(−33, −.33)	(−.2, .3)	(−.1, .4)	(.0, .5)	(.1, .6)
m=4	x_2	−.7365	−.7065	−.6783	−.6513	−.6256
	x_3	−.2732	−.2112	−.1406	−.0731	−.0083
	x_4	.2732	.2841	.3555	.4249	.4925
	x_5	.7365	.7359	.7659	.7965	.8281
m=5	x_2	−.8179	−.8006	−.7838	−.7678	−.7524
	x_3	−.4541	−.4121	−.3663	−.3219	−.2788
	x_4	.0	−.0309	.0927	.1548	.2173
	x_5	.4541	.4598	.5095	.5616	.6161
	x_6	.8179	.8181	.8367	.8565	.8777
m=6	x_2	−.8666	−.8551	−.8441	−.8336	−.8238
	x_3	−.5840	−.5537	−.5215	−.4909	−.4619
	x_4	−.2083	−.1729	−.1214	−.0713	−.2276
	x_5	.2083	.2252	.2778	.3306	.3836
	x_6	.5840	.5876	.6233	.6610	.7010
	x_7	.8666	.8669	.8796	.8931	.9079

References

[1] de Boor, C.(1978). *A Practical Guide to Splines*. Springer-Verlag, New York.

[2] Fedorov, V.V.(1972). Theory of Optimal Experiments, Translated by W.J. Studden & E.M. Klimko. Academic Press, New York.

[3] Kiefer, J. and Wolfowitz, J.(1960). "The Equivalence of Two Extremum Problems," *Canad. J. Math.*, Vol. 12, 363-366.

[4] Lim, Y.B.(1986). Optimal Designs in Multivariate Polynomial Regression and Polynomial Spline Regression. Ph.D. Thesis, Purdue University.

[5] Murty, V.N.(1971). "Optimal Designs with a Polynomial Spline Regression with a Single Multuple Knot at the Center," *Ann. Math. Statist.*, Vol. 42, 952-960.

[6] Park, S.H.(1978). "Designs for Fitting Segmented Polynomial Regression Models," *Technometrics*, Vol. 20, 151-154.

[7] Schumaker, L.L.(1981). *Spline Functions: Basic Theory*. John Wiley & Sons, New York.

[8] Studden, W.J.(1971). "Optimal Designs and Spline Regression," *In Optimizing Methods in Statistics*, 63-75, Academic Press, New York.

[9] Studden, W.J. and Van Arman, D.J.(1969). "Admissible Designs for Polynomial Spline Regression," *Ann. Math. Statist.*, Vol. 40, 1557-1569.

[10] Welch, W.J.(1985). "ACED: Algorithms for the Construction of Experimental Designs," *Am. Statist.*, Vol. 39, 146.

[11] Wynn, H.P.(1970). "The Sequential Generation of D-optimal Designs," *Ann. Math. Statist.*, Vol. 41, 1655-1664.

다항 스플라인 회귀모형에서의 D－최적실험계획†

임 용 빈*

요 약

고정된 접목점을 갖는 다항 스플라인 회귀모형에 대한 D－최적실험 계획의 성질들이 연구되었다. 또한 정규화된 B－스플라인을 이용하여 몇가지 경우에 대한 D－최적실험 계획을 이론적으로 구하였다. Kiefer－Wolfowitz 동치정리에 의하여 몇가지 모형에 대한 D－최적실험 계획이 수리적인 방법에 의해 근사적으로 구하여 졌다.

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