Classification of Experimental Designs Relative to Polynomial Spline Regression Functions

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INTRODUCTION

Let $\overline{f}(x)=(f_0(x),\ldots,f_m(x))^T$ be a vector of linearly independent continuous functions on [a,b]. We assume that for each x or ''level'' in [a,b] an experiment can be performed whose outcome is a random variable Y(x) and that for any x, var Y(x)=1. Also assumed is the existence of $\overline{\theta}=(\theta_0,\ldots,\theta_m)^T$ such that $E(x)=(\overline{f}(x),\overline{\theta})$. The functions f_0,\ldots,f_m are called the regression functions and assumed known to the experimenter. The basic problem is the estimation of functions of the vector $\overline{\theta}$ by means of a finite number N of uncorrelated observations, $\{Y(x_i)\}_{i=1}^N$. Thus, given a criterion of what a good estimate of a certain $g(\overline{\theta})$ is, the problem is one of selecting the x_i 's at which to experiment.

An experimental design is a probability measure μ that has mass p_1, \ldots, p_r on the points x_1, \ldots, x_r respectively, where p_i $N=n_i$, an integer. An experimental design determines the points at which the experiment takes place, namely the x_i , $i=1,\ldots,r$, and the number of experiments at each level, namely n_i at x_i .

Definition 1: Let μ be an arbitrary probability measure on [a,b]. $M(\mu)$, the information matrix of μ , is defined as $||m_{ij}(\mu)||_{i,j=0}^m$, where $m_{ij}(\mu) = \int_{[a,b]} f_i(x) f_j(x) d\mu(x)$.

Notice that the information matrix is clearly non-negative definite.

The information matrix plays an important role in determining the accuracy of estimates to certain $g(\overline{\Theta})$. Consider the problem of unbiased

estimation of $(\overline{c}, \overline{\theta})$, where \overline{c} is some m+l vector of constants. Let a design $\mu = \{x_i, p_i\}_{i=1}^r$ be given, where $p_i N = n_i$. The experimenter has N random variables to work with, $Y_1(x_1), \dots, Y_{n_1}(x_1), \dots, Y_1(x_r), \dots, Y_{n_m}(x_r)$. is known (see e.g., Karlin and Studden, 1966a) that if there exists a linear unbiased estimate of (c, θ) in terms of these random variables, there exists one of minimum variance and that this minimum variance is precisely $\frac{1}{N} \sup_{\overline{d} \in U_{\perp}} \frac{(\overline{c}, \overline{d})^2/(\overline{d}, M(\mu)\overline{d})}{\overline{d} \in U_{\perp}} = {\overline{d} \mid M(\mu)\overline{d} = 0}.$ The crucial quantum of the crucial tity in this expression is $V(\overline{c},\mu) = \sup_{\overline{d} \in U^{\perp}} \frac{(\overline{c},\overline{d})^2}{(\overline{d},M(\mu)\overline{d})}$. Assume that there is a μ ' such that $M(\mu^{\,\prime})-M(\mu)$ is non-negative definite. Then it is also known that there is μ' concentrated on a finite set of points in [a,b] with this property (see Lemma 1). For this μ' , $V(c,\mu')$ will be at least as small as $V(\overline{c},\mu)$. This follows because the existence of a linear unbiased estimate of $(c, \overline{\theta})$ with respect to μ is equivalent to c being in U_{ij}^{\perp} (see Karlin and Studden, 1966a) and thus in U_{μ}^{\perp} , U_{μ}^{\perp} being contained in U_{μ}^{\perp} . If μ ' is not an experimental design, i.e., if μ ' has irrational weight at some point, it can still be viewed as an approximate experimental design for large N. With this outlook we can think of μ ' as giving a better best variance than μ for linear unbiased estimates of $(\overline{c}, \overline{\theta})$.

Definition 2: Let μ and μ' be probability measures on [a,b]. We say $\mu \leq \mu'$ or $M(\mu) \leq M(\mu')$ if the matrix $M(\mu')$ - $M(\mu)$ is non-negative definite and unequal to the 0 matrix.

<u>Definition 3</u>: A probability measure μ is said to be admissible if there is no probability measure μ' such that $\mu' \geq \mu$. Otherwise μ is inadmissible.

Because inadmissible designs give bigger variances than their dominating designs and because every inadmissible design is dominated by an admissible design (see Lemma 3), we are interested in determining the class of admissible designs.

Definition 4: Let μ be a probability measure on [a,b] concentrated on $\{x_1,\ldots,x_r\}$ such that $\mu(x_i)>0,i=1,\ldots,r$. Then the set $\{x_1,\ldots,x_r\}$ is called the spectrum of μ , written $S(\mu)$.

It is known that admissibility is a property of the spectrum of a measure (see Lemma 2), that is, if μ_1 and μ_2 have the same spectrum they are either both admissible or both inadmissible. Thus we can speak of admissible or inadmissible spectra.

When $\overline{f}(x) = (1,x,\ldots,x^n)^T$ it is known that a spectrum in $\lceil a,b \rceil$ is admissible if and only if it contains no more than n-1 points in the open interval (a,b) (see Theorem 2). Many other results are known in this case. For example, if we let $C = \{\overline{c} \mid \overline{c} = (1,x,\ldots,x^n)^T \text{ for } x \in [a,b]\}$, then the design concentrating equal mass on the zeros of $(1-x^2) P_n'(x) (P_n(x))$ is the nth Legendre polynomial) is minimax in the sense that it minimizes $\sup_{c \in C} V(\overline{c},\mu)$ (see Kiefer, 1959). Hoel and Levine (1964) have investigated the design which minimizes $V(\overline{c},\mu)$ for $\overline{c} = (1,x_0,\ldots,x_0^n)$ and $x_0 \notin [a,b]$, an extrapolation problem. Extensions and modifications of this problem are considered in Kiefer and Wolfowitz (1964, 1965) and Studden (1968).

The problem attacked in this thesis is that of characterizing admissible designs when the regression vector $\overline{f}(x)$ is in the following form

(1)
$$(1,x,...,x^n, (x-\xi_1)_+^{n-k},...,(x-\xi_1)_+^n,...,(x-\xi_h)_+^{n-k},...,(x-\xi_h)_+^n)^T$$

where a $< \xi_1 < \ldots < \xi_h <$ b, $0 \le k \le n-1$ and where

$$(x-\xi)_{+}^{m} = \begin{cases} 0, & x < \xi \\ & , & m = 1,2,... \end{cases}$$

A polynomial in the component functions of $\overline{f}(x)$ is called a polynomial spline function with knots at F_1, \dots, F_h . A function has this form if and only if it is a regular polynomial on $(a, F_1), (F_1, F_2), \dots, (F_h, F_h)$ and n-k-1 times differentiable at the knots F_1, \dots, F_h (see Lemma 4). Spline functions have received considerable attention from mathematicians working in numerical analysis, interpolation and approximation theory. (See Schoenberg, 1964 and Karlin, 1968 for further references).

Chapter I will start off by discussing some of the basic results upon which this work is dependent. Section 1 has general lemmas about information matrices, spline polynomials, and admissibility. It also reviews what is known in the polynomial case. The rest of Chapter I deals with the problem of determining the admissible spectra in the case of one knot, i.e., when $\overline{f}(x) = (1,x,\ldots,x^n, (x-\xi)^{n-k}_+,\ldots,(x-\xi)^n_+)^T$. Section 2 gives necessary and sufficient moment conditions for admissibility. Section 3 uses a result by Karlin and Ziegler to get some properties of spline functions for later use. Section 4 starts by applying what is known about the polynomial case to the spline polynomial case to determine a large class of inadmissible designs. Then the results of Section 3 are used to classify another large class of spectra, leaving only a few cases undetermined. In Section 5 these undetermined designs are classified by theorems that overlap some of the theorems of Section 4. The final result is that a design is admissible

relative to $\overline{f}(x) = (1,x,...,x^n,(x-\xi)_+^{n-k}+,...,(x-\xi)_+^n)^T$ if and only if

- (1) $S(\mu)$ has fewer than n points in (a,ξ) and (ξ,b) and
- (2) $S(\mu)$ has fewer than $n + \frac{n+k}{2}$ points in (a,b).

In Chapter II we consider the case of h knots, where the regression vector is $\overline{f}(x) = (1, x, ..., x^n, (x-\xi_1)_+^{n-k}, ..., (x-\xi_1)_+^n, ..., (x-\xi_h)_+^{n-k}, ...,$ $(x-\xi_h)_+^n)^T$. The first section generalizes Theorem 3, again giving admissibility in terms of moment conditions. Section 2 contains a generalization of Theorem 4, using what is known about the problem for fewer than h knots and applying it to the case of h knots. We see that if μ is inadmissible with respect to fewer than h knots, then μ can't be admissible for h In Section 3, we see that a design is admissible if it is subadmiss-1ble (i.e., admissible for fewer than h knots) and has few enough points $[a,\xi_1)$ or $(\xi_h,b]$. We also give some examples in Section 3, one of which classifies all designs in the case when k = n-1. In this case, where the regression function is such that it need only be continuous at the knots, a design is admissible if and only if it has no more than n-l points in each of the intervals (a,ξ_1) , (ξ_h,b) and (ξ_i,ξ_{i+1}) , $i=1,\ldots,h-1$. Section 4 we consider the case of a second differentiable regression function, i.e., where k = n-2, and succeed in characterizing a large class of designs as inadmissible. We show that designs with n+h(n-1) or more points in (a,b) are inadmissible. We also show that subadmissible designs with (h+1)(n-1) or fewer points in (a,b) are admissible when none of these points are at the knots. Section 5 conjectures that the remaining subadmissible designs with (h+1)(n-1) or fewer points in (a,b) are admissible. It also offers a conjecture for the general solution of the problem, that

than $n+h(\frac{n+k}{2})$ points in (a,b) - unless it is subadmissible and has $\frac{n+k-1}{2}$ or fewer points in (ξ_h,b) or (a,ξ_1) ; then it is admissible. Section 6 mentions how Theorems 3 and 10 and Lemmas 8 and 16 can be generalized for the case where the regression function is arbitrarily differentiable at the knots, i.e., where $\overline{f}(x)=(1,x,\ldots,x^n,(x-\xi_1)^n_+,\ldots,(x-\xi_1)^n$

CHAPTER I

CHARACTERIZATION OF ADMISSIBLE DESIGNS

IN THE CASE OF ONE KNOT

1. Some Background Lemmas

In this section we present some fundamental results that are relevant to this thesis, the first lemma describing some basic properties of information matrices.

<u>Lemma 1.</u> Let $\overline{f}(x) = (f_0(x), \dots, f_m(x))^T$ and let $M(\mu)$ be as in Definition 1. Then

- (1) $M(\mu)$ is non-negative definite;
- (2) det $M(\mu)$ = 0 if all the mass of μ is concentrated on fewer than m+l points;
- (3) the family of matrices $\{M(\mu)\}$, for μ a probability measure, is a convex compact set;
- (4) for each μ there is a probability measure μ ' concentrated on r points, $r \leq \frac{(m+1)(m+2)}{2} + 1$, such that $M(\mu) = M(\mu')$.

Proof: See Karlin and Studden (1966a, p. 787).

The far reaching part of this lemma is part (4) which permits us to restrict attention to measures concentrated on a finite set of points when dealing with information matrices. Since our criterion of admissibility is given in terms of information matrices, we henceforth restrict consideration to measures on a finite set of points.

Lemma 2. Let μ be an admissible measure concentrated on $\{x_1, \dots, x_r\}$ with weight $p_i > 0$ at x_i . Then if μ' is a measure concentrated on $\{x_1, \dots, x_r\}$ with weight $q_i \geq 0$ at x_i , μ' is admissible.

Proof: See Karlin and Studden (1966a, p. 809).

This lemma tells us that any measure concentrated on a subset of the spectrum of an admissible spectrum is admissible, or that a subspectrum of an admissible spectrum is admissible. It also tells us that if μ is inadmissible, a measure whose spectrum is a superspectrum of $S(\mu)$ is inadmissible, or that a superspectrum of an inadmissible spectrum is inadmissible. Thus we can talk of admissible and inadmissible spectra from now on.

The next lemma is the one that guarantees that we get best linear unbiased estimation results by staying in the admissible class of designs.

<u>Iemma 3.</u> Let μ be an inadmissible measure. Then there is an admissible μ' such that $\mu' \geq \mu$.

Proof: We start by noting that any $M(\mu') \geq M(\mu)$ has its main diagonal elements greater than or equal to the corresponding diagonal terms of $M(\mu)$ and that at least one must be strictly bigger (see Lemma 7). Let $\alpha_1 = \sup_{\mu' \geq \mu} \quad (m_{11}(\mu')).$ By compactness of $\{M(\mu)\}$ (Lemma 1) there is a $\mu' \geq \mu$ $M(\mu'_1)$ such that $m_{11}(\mu'_1) = \alpha_1$ and $M(\mu'_1) \geq M(\mu).$ If μ'_1 is admissible we are done. If not we let $\alpha_2 = \sup_{\mu' \geq \mu'_1} \quad (m_{22}(\mu'))$ and notice there is a $\mu' \geq \mu'_1 \quad \text{is admissible we are done. Proceeding in this way we either arrive at an admissible <math>M(\mu'_1)$, for i < m+1, or we arrive at an $M(\mu'_{m+1})$ with the properties that $\alpha_j = m_{j,j}(\mu'_{m+1}), \quad j=1,\ldots,m+1$ and $M(\mu'_{m+1}) \geq M(\mu'_m) \geq \ldots \geq M(\mu'_1) \geq M(\mu).$ By the preliminary

remark, if there is a $\hat{\mu} \geq \mu'_{m+1}$, $m_{kk}(\hat{\mu}) > m_{kk}(\mu'_{m+1})$ for some k contradicting the meaning of α_k . Thus $M(\mu'_{m+1})$ must be admissible.

The next lemma is a formal characterization of the type of regression function we are interested in.

Lemma 4. A function P(x) on [a,b] can be expressed in the form

(2)
$$P(x) = \sum_{i=0}^{n} b_{i} x^{i} + \sum_{i=1}^{n} \sum_{j=0}^{k} a_{ij} (x-\xi_{i})_{+}^{n-j}$$

if and only if

- (1) P(x) is a regular polynomial in each of the intervals $[a,\xi_1),(\xi_1,\xi_2),\ldots,(\xi_{h-1},\xi_h),(\xi_h,b]$ and
- (2) P(x) is of continuity class n-k-l at each ξ_i , i.e., it has n-k-l continuous derivatives at ξ_i .

Proof: See Karlin and Ziegler (1966, p. 518).

Sometimes in the ensuing analysis it will be easiest to work with a linear transformation of the regression vector (1).

<u>Lemma 5.</u> Let $\overline{g}(x) = A\overline{f}(x)$ where A is non-singular and where $\overline{f}(x)$ is given in (1). Then a design μ is admissible with respect to $\overline{g}(x)$ if and only if it is admissible with respect to $\overline{f}(x)$.

Proof: Notice that for any v,

$$\underline{\underline{M}}_{g}(v) = \int_{[a,b]} A\overline{f}(x) \overline{f}^{T}(x) A^{T} dv = A\underline{\underline{M}}_{f}(v) A^{T}.$$

Let μ be admissible with respect to $\overline{f}(x)$. Then if μ is not admissible with respect to $\overline{g}(x)$ there exists a ν such that $\nu \geq \mu$ with respect to

 $\overline{g}(x)$ or $AM_{\overline{f}}(v) A^{\overline{T}} \geq AM_{\overline{f}}(\mu) A^{\overline{T}}$. Since A is non-singular, this implies $M_{\overline{f}}(v) \geq M_{\overline{f}}(\mu)$. So μ must be admissible with respect to $\overline{g}(x)$. The ''only if'' part follows from the same argument upon noting $\overline{f}(x) = A^{-1}\overline{g}(x)$.

Remark. If we are only considering the case of one knot ξ , where $\overline{f}(x) = (1,x,\ldots,x^n, (x-\xi)_+^{n-k}+\ldots,(x-\xi)_+^n)^T$, we can define $(x-\xi)_-^m=(x-\xi)_-^m-(x-\xi)_+^m$, $m=1,2,\ldots$ and let $\overline{g}(x) = (1,x,\ldots,x^n,(x-\xi)_-^{n-k},\ldots,(x-\xi)_-^n)^T$. It can be observed that $\overline{g}(x)$ is a non-singular linear transformation of $\overline{f}(x)$ and thus that a measure is admissible with respect to one vector if and only if it is admissible with respect to the other.

We now state a result due to Kiefer (1959, p. 291) that is instrumental in characterizing the admissible spectra in the ordinary polynomial case, when $\overline{f}(x) = (1, x, ..., x^n)^T$. We will use a generalization of his theorem to attack the spline polynomial case.

Theorem 1. Let $\overline{f}(x)=(1,x,\ldots,x^n)^T$ and let $\overline{g}(x)=(1,x,\ldots,x^{2n-1})^T$. Then $\mu'\geq \mu$ if and only if

(1)
$$\int_{[a,b]} \overline{g}(x) d(\mu'-\mu) = 0 \text{ and}$$

(2)
$$\int_{[a,b]} x^{2n} d(\mu' - \mu) > 0.$$

Proof: See Karlin and Studden (1966 b, p. 352).

Following closely after Kiefer's ''momentous'' result is the theorem that characterizes the admissible spectra.

Theorem 2. Let $\overline{f}(x)$ be as above. A probability measure μ on [a,b] is admissible if and only if its spectrum has fewer than n points in the open interval (a,b).

Proof: See Karlin and Studden (1966b, p. 353).

The proof essentially depends upon recognizing the fact that $\int_{[a,b]}^{x^{2n}} d\mu$ is maximal subject to the prior moments being fixed if and only if μ is a measure with fewer than n mass points in (a,b). The method of approach used in the spline polynomial case is similar, only the analysis more delicate and complicated. The result is similar, that a design is admissible if and only if its spectrum has fewer than a certain number of points in certain intervals.

2. A Necessary and Sufficient Condition for Admissibility

We now develop a generalization of Kiefer's theorem, again showing admissibility related to certain moment conditions.

Lemma 6. If

$$M = \begin{pmatrix} a & b \\ b & b \end{pmatrix},$$

 $M \ge 0$ if and only if $0 \neq a \ge b \ge 0$.

Proof: This can be observed after noting

$$(x,y) M(_y^x) = x^2(a-b)+b(x+y)^2.$$

Lemma 7. Suppose M is symmetric and $M \ge 0$. If a diagonal element $m_{i,j} = 0$, then $m_{i,j} = 0$ for all j.

Proof: Let \overline{v} be the vector with 1 in the ith place, β in the jth place, and 0's elsewhere. Then for all β ,

$$\overline{v}$$
 \overline{v} \overline{v} = $2\beta m_{i,j} + \beta^2 m_{j,j} \ge 0$.

Thus for all $\beta > 0$,

$$(2m_{i,j} + \beta m_{j,j}) \ge 0.$$

Letting $\beta \downarrow 0$ we have $2m_{i,j} \geq 0$. Also for all $\beta < 0$,

$$(2m_{ij} + \beta m_{jj}) \leq 0.$$

Letting β † 0 we get $2m_{i,j} \le 0$. Thus $m_{i,j} = 0$.

Theorem 3. Let $\overline{f}(x) = (1,x,\ldots,x^n,(x-\xi)_+^{n-k},\ldots,(x-\xi)_+^n)^T$. Let $\overline{g}(x) = (1,x,\ldots,x^{2n-1},(x-\xi)_+^{n-k},\ldots,(x-\xi)_+^{2n-1})^T$. Then with respect to the regression vector $\overline{f}(x)$, $M(\mu')-M(\mu) \geq 0$ if and only if

(1)
$$\int \overline{g}(x) d(\mu' - \mu) = 0$$
 and

(2)
$$0 \neq \int x^{2n} d(\mu' - \mu) \geq \int (x - \xi)^{2n} d(\mu' - \mu) \geq 0.$$

Proof: Let $m_{i,j}$ be the (i,j) element of the symmetric matrix $M = M(\mu') - M(\mu)$. Assume $M \geq 0$. We will show (1) holds by repeated application of Lemma 7. Since

$$\int 1 d\mu = \int 1 d\mu'$$

or $m_{11} = 0$, the first row and column of M are 0. That is,

(a)
$$\int x^{i} d(\mu' - \mu) = 0$$
, $i = 0,...,n$ and

(b)
$$\int (x-\xi)^{\frac{1}{2}} d(\mu'-\mu) = 0$$
, $j = n-k,...,n$.

Statement (a) tells us $m_{22} = \int x^2 d(\mu' - \mu) = 0$, so that the second row and column are 0, or

$$\int x^{i} d(\mu'-\mu) = 0$$
, $i = 1,...,n+1$

and

$$\int x(x-\xi)_{+}^{j} d(\mu'-\mu) = 0, \quad j = n-k,...,n.$$

Continuing this way we finally arrive at

(c)
$$\int x^{i} d(\mu' - \mu) = 0$$
, $i = 0,...,2n-1$ and

(d)
$$\int x^{i}(x-\xi)^{j}_{+} d(\mu'-\mu) = 0$$
, $i = 0,...,n-1$, $j = n-k,...,n$.

Since for i = 0, ..., n-1 and j = n-k, ..., n

$$\int (x-\xi)^{\frac{1}{4}} (x-\xi)^{\frac{1}{4}} d(\mu'-\mu) = \sum_{k=0}^{1} a_{k} \int x^{k} (x-\xi)^{\frac{1}{4}} d(\mu'-\mu) = 0,$$

by (d), we get

$$\int (x-\xi)^{\frac{1}{2}} d(\mu'-\mu) = 0, \quad i = n-k,...,2n-1.$$

Thus $M \ge 0$ implies (1).

We notice that when (1) holds M has its first n and then its n+2,..., n+k+1 st rows and columns O. That is, (1) implies the elements of M other than $m_{n+1,n+1} = \int x^{2n} d(\mu' - \mu)$, $m_{n+k+2,n+k+2} = \int (x-\xi)^{2n}_+ d(\mu' - \mu)$, and $m_{n+1,n+k+2} = m_{n+k+2,n+1} = \int x^n (x-\xi)^n_+ d(\mu' - \mu)$ are O. We notice that (1) also implies

$$\int x^{n}(x-\xi)^{n}_{+} d(\mu'-\mu) = \int (x-\xi)^{2n}_{+} d(\mu'-\mu)$$

since

$$x^{n}(x-\xi)_{+}^{n} = (x-\xi)^{n}(x-\xi)_{+}^{n+} + \sum_{k=0}^{n-1} a_{k}(x-\xi)^{k}(x-\xi)_{+}^{n} = (x-\xi)_{+}^{2n} + \sum_{k=0}^{n-1} a_{k}(x-\xi)_{+}^{n+k}.$$

Thus $m_{n+k+2,n+k+2} = m_{n+1,n+k+2} = m_{n+k+2,n+1}$. Finally, by Lemma 6, assuming (1), $M \ge 0$ if and only if (2) holds. This completes the proof.

Corollary. If μ is admissible when k = m, μ is admissible when k > m, m = 1,...,n-2, m < k \leq n-1.

Proof: One need only observe that if μ' dominates μ for k>m, μ' dominates μ for k=m.

We now state Theorem 3 in an equivalent but slightly more general and usable way.

Theorem 3'. Let $\overline{g}_1(x) = (1, x, \dots, x^{2n-1}, (x-\xi)_-^{n-k}, \dots, (x-\xi)_-^{2n-1})^T$ and let $\overline{g}_2(x) = (1, x, \dots, x^{2n-1}, (x-\xi)_+^{n-k}, \dots, (x-\xi)_+^{2n-1})^T$. Then with respect to the regression vector $f_1(x) = (1, x, \dots, x^n, (x-\xi)_+^{n-k}, \dots, (x-\xi)_+^n)^T$ or $\overline{f}_2(x) = (1, x, \dots, x^n, (x-\xi)_-^{n-k}, \dots, (x-\xi)_-^n)^T$ (see Lemma 5 and Remark) $M(\mu') \geq M(\mu)$ if and only if

(1)'
$$\int_{\overline{g}_{1}}(x) d(\mu' - \mu) = 0$$
 or

$$\int_{\mathbb{F}_{2}} (x) d(\mu' - \mu) = 0 \quad \text{and} \quad$$

(2)'
$$\int (x-\xi)^{2n}_{+} d(\mu'-\mu) \ge 0$$
 and
$$\int (x-\xi)^{2n}_{-} d(\mu'-\mu) \ge 0$$

and one of the inequalities is strict.

Proof: Notice that conditions (1)' and (1) are equivalent and that given (1)', condition (2)' is equivalent to condition (2).

Lemma 5 and Theorem 3' show some of the symmetry that is inherent in the situation. Later we shall prove certain things by showing one case and claiming another case is true by symmetry.

3. Some Characteristics of Spline Functions

In this section we present two lemmas dealing with spline polynomials that will permit us to ''weave'' polynomials through questionable spectra. First we paraphrase a result of Karlin and Ziegler (1966, pp.519-22).

Let $\varphi_m(t,x) = (t-x)_+^m$, m = 1,2,... and let t_i , x_j , i,j = 1,2,...,r, satisfy conditions (1), (2), and (3):

- (1) $c \le t_1 \le \dots \le t_r \le d$, $c \le x_1 \le \dots \le x_r \le d$;
- (2) $\alpha+\beta\leq s+2$ ($s\geq 1$) whenever α of the x_j 's, $1\leq \alpha$, coincide, say equal to g, $c\leq g\leq d$, and β of the t_i 's, $1\leq \beta$, agree with the same point g.
- (3) No more than s+l consecutive t's (or x's) coincide. Let $M(s,\overline{t},\overline{x})$ be defined as follows: If $x_1 < x_2 < \dots < x_r$ and $t_1 < t_2 < \dots < t_r$, $M(s,\overline{t},\overline{x})$ is the matrix $||\phi_s(t_i,x_j)||_{i,j=1}^r$. If $x_j < x_j < x_j$

A similar adjustment is used on the rows of the resultant matrix when t values coincide, any sth derivative being taken from the right. $M(s,\overline{t},\overline{x})$ is the remaining matrix. We let $D(s,\overline{t},\overline{x})$ be defined as det $M(s,\overline{t},\overline{x})$. The result of Karlin and Ziegler is that under conditions (1), (2), and (3) $D(s,\overline{t},\overline{x}) \geq 0 \quad \text{always and} \quad D(s,\overline{t},\overline{x}) > 0 \quad \text{if and only if} \quad t_{i-(s+1)} < x_{i} < t_{i}, \quad t_{i-(s+1)} < x_{i} < t_{i-(s+1)} < x_{i} < t_{i-(s+1)} < x_{i-(s+1)} < x_{i-(s+1$

<u>Definition 5.</u> Let $\overline{f}(x)$ be a vector of functions $(f_1(x), \dots, f_h(x))^T$ and let \overline{t} be a vector of constants $(t_1, \dots, t_h)^T$ where $t_1 \le t_2 \le \dots \le t_h$.

Then for $t_1 < t_2 < \dots < t_h$ we let $M(\overline{f}, \overline{t})$ be a matrix $M_o = (\overline{f}(t_1), \dots, \overline{f}(t_h))$. Otherwise, if t values coincide, say $t_{i_o} - 1 < t_{i_o} = t_{i_o} + 1 = \dots = t_{i_o} + j - 1 < t_{i_o} + j$, we let $M(\overline{f}, \overline{t})$ be the matrix obtained by replacing the $i_o + k$ th column, $k = 1, \dots, j - 1$, of M_o by the vector $\left[\frac{d(k)}{dt^k} \overline{f}(t)\right|_{t=t_{i_o}}$, where all derivatives

are from the right.

We now apply the Karlin-Ziegler result with $r=s+\ell+2$, $0 \le \ell \le s-1$, $c=a-\epsilon$, d=b, $x_1=\cdots=x_{s+1}=a-\epsilon$, and $x_{s+2}=\cdots=x_{s+\ell+2}=\xi$. We notice $D(s,\overline{t},\overline{x}) \neq 0$ if and only if $t_{\ell+1} \le \xi$ and $t_{s+2} > \xi$.

Lemma 8. Let $\overline{f}(x) = (1,x,...,x^s, (x-\xi)_+^{s-\ell},...,(x-\xi)_+^s)^T$. Let $a \le t_1 \le ... \le t_{s+\ell+2} \le b$ where no more than $(s-\ell+1)$ t values are ξ and where no more than (s+1) t values coincide. Then $M(\overline{f},\overline{t})$ is non-singular if and only if there are no more than (s+1) t values in both [a,b] and $[\xi,b]$.

Proof: We need only note

(3)
$$M^{T}(\overline{f},\overline{t}) = M(s,\overline{t},\overline{x}) \begin{bmatrix} M_{1} & O \\ O & M_{2} \end{bmatrix}$$

where M_1 is an (s+1)x(s+1) non-singular lower right triangular matrix of constants and where M_2 is an $(\ell+1)x(\ell+1)$ non-singular non-principle diagonal matrix of constants. Then det $M(\overline{f},\overline{t}) \neq 0$ if and only if $D(s,\overline{t},\overline{x}) \neq 0$ or if and only if $t_{\ell+1} < \xi$ and $t_{s+2} > \xi$.

<u>Lemma 9.</u> Let $\ell < s$ and $a \le t_1 \le \dots \le t_{s+\ell+1} \le b$, where $t_{s+1} > \xi$ and $t_{\ell+1} < \xi$. Then there is a non-trivial polynomial unique up to a multiplicative constant in the components of $\overline{f}(x) = (1, x, \dots, x^s, (x-\xi)_+^{s-\ell}, \dots, (x-\xi)_+^s)^T$ with 0's at the t_i 's. (If h t_i 's agree with some point, we mean the 0 at

this point will have multiplicity h.) Furthermore this polynomial has no other 0's in $(-\infty,\infty)$.

Proof: Let $t_{s+\ell+2} = b+1$ and let $\overline{t} = (t_1, \dots, t_{s+\ell+1}, t_{s+\ell+2})^T$. By Lemma 8, $M(\overline{f}, \overline{t})$ is non-singular and there is a unique $\overline{\alpha}$ such that $M^T(\overline{f}, \overline{t})\overline{\alpha} = (0,0,\dots,0,1)^T$. Thus there is a unique polynomial $P(x) = (\overline{f}(x), \overline{\alpha})$ with 0's at $t_1,\dots,t_{s+\ell+1}$ such that $P(t_{s+\ell+2}) = 1$. Notice that the condition that $t_{\ell+1} < \xi$ and $t_{s+1} > \xi$ implies at most $(s-\ell-1)$ t's fall on ξ and that we need not worry about an extended definition of ''multiplicity'' (see Definition 8). We now show that P(x) has no other 0's on $(-\infty,\infty)$. Assume there is some other 0, say t_0 . Let \overline{t} be the vector with components $t_0, t_1, \dots, t_{s+\ell+1}$ in monotone non-decreasing order. Then no matter where t_0 is, $M(\overline{f}, \overline{t})$ is still non-singular by Lemma 8. Since $M^T(\overline{f}, \overline{t})\overline{\alpha} = \overline{0}$ has a unique solution $\overline{\alpha} = 0$, we note that the only polynomial with 0's at $t_0, \dots, t_{s+\ell+1}$ is the trivial one.

4. Weak Bounds on the Spectrum

We start this section by applying what we know about the regular polynomial case (Theorem 2) to the spline polynomial case. Then we prove two theorems giving bounds on the number of points in admissible and inadmissible spectra. These theorems are later superceeded by other theorems which give better bounds from independent arguments; but the theorems of this section are interesting because they help one see why μ is inadmissible if $S(\mu)$ is too big and admissible if $S(\mu)$ is small enough.

Theorem 4. Let $f(x) = (1, x, ..., x^n, (x-\xi)_+^{n-k}, ..., (x-\xi)_+^n)^T$. If $S(\mu)$ has more than n-l points in either (a,ξ) or (ξ,b) , then μ is inadmissible with respect to $\overline{f}(x)$.

Proof: First consider the case when $S(\mu)$ has more than n-l points in (a,ξ) . Let $\hat{\mu}=\frac{\mu}{\mu[a,\xi]}$ on $[a,\xi]$. By Theorem 2, $\hat{\mu}$ is inadmissible on $[a,\xi]$ relative to the regression vector $\overline{g}(x)=(1,x,\ldots,x^n)^T$. Thus there is a $\hat{\mu}'$ on $[a,\xi]$ such that $M(\hat{\mu}')\geq M(\hat{\mu})$ (relative to $\overline{g}(x)$). Let

$$\mu' = \begin{cases} \mu[a,\xi] \hat{\mu}' & \text{on } [a,\xi] \\ \mu & \text{on } (\xi,b] \end{cases}.$$

We notice

$$M(\mu) = \int_{[a,\xi]} \overline{f}(x) \overline{f}^{T}(x) d\mu + \int_{\{\xi,b\}} \overline{f}(x) \overline{f}^{T}(x) d\mu$$

and

$$M(\mu') = \int_{[a,\xi]} \overline{f}(x) \overline{f}^{T}(x) d\mu' + \int_{[\xi,b]} \overline{f}(x) \overline{f}^{T}(x) d\mu.$$

Since

$$\int_{\left[a,\xi\right]} \overline{f}(x) \ \overline{f}^{T}(x) \ d\mu' \geq \int_{\left[a,\xi\right]} \overline{f}(x) \ \overline{f}^{T}(x) \ d\mu,$$

 $\texttt{M}(\mu^{\, \text{!`}}) \, \geq \, \texttt{M}(\mu) \,$ and μ is inadmissible.

In the case where $S(\mu)$ has more than n-l points in (ξ,b) the result follows from a symmetric argument.

The next definition is motivated by Theorem 4.

<u>Definition 6.</u> Let $I(\mu) = +\infty$ if $S(\mu)$ has more than n-1 points in either (a,ξ) or (ξ,b) . Otherwise let $I(\mu)$ be the number of interior points of [a,b] in $S(\mu)$ plus one-half the number of end points of [a,b]

in $S(\mu)$, if any. $I(\mu)$ will be called the index of μ .

As suggested above $\,\mu$ will be inadmissible if $I(\mu)\,$ is too big and $\,\mu$ will be admissible if $\,I(\mu)\,$ is small enough.

 $\underline{\text{Lemma 10}}. \quad \text{Let } \overline{g}(t) = (1,t,\ldots,t^{2n-1},\; (t-\xi)_+^{n-k},\ldots,(t-\xi)_+^{2n-1})^T \quad \text{and} \\ \text{assume } I(\mu) < \infty. \quad \text{Then if } \int \overline{g}(t) \; d(\mu'-\mu) = 0 \quad \text{and } S(\mu') \subset S(\mu),\; \mu' = \mu.$

Proof: Consider the elements of $S(\mu)$ as being ordered from a to b and suppose $S(\mu') \subset S(\mu)$. Then let $\overline{\theta}$ be the vector of weights of μ , the ith component of $\overline{\theta}$ being the μ weight of the ith element of $S(\mu)$. Let $\overline{\theta}'$ be the vector whose ith component is the μ' weight of the ith element of $S(\mu)$. Let M be the matrix whose ith column is $\overline{g}(t_i)$ where t_i is the ith element of $S(\mu)$. Then $\int \overline{g}(t) \ d(\mu' - \mu) = 0$ implies $M(\overline{\theta} - \overline{\theta}') = \overline{0}$. Since, by Lemma 8, the columns of M are independent, $\overline{\theta} - \overline{\theta}' = 0$ and $\mu' = \mu$.

Theorem 5. If $I(\mu) \leq \frac{3n+k-1}{2}$, then μ is admissible.

Proof: Case 1, $I(\mu) = \frac{3n+k-1}{2}$ and there are fewer than n points of $S(\mu)$ in $(a,\xi]$ and $[\xi,b)$. Then with s=2n-1 and $\ell=n+k-1$, Lemma 9 tells us there is a non-trivial polynomial P(x) in $1,x,\ldots,x^{2n-1}$, $(x-\xi)^{n-k}_+,\ldots,(x-\xi)^{2n-1}_+$ with a single 0 at each end point of [a,b] in $S(\mu)$, a double 0 at each interior point of [a,b] in $S(\mu)$, and no other 0's, so that P(x) has constant sign on [a,b]. If there were a $\mu' \geq \mu$, Theorem 3, part 1,tells us $\int P(x) \ d\mu' = \int P(x) \ d\mu = 0$ and thus that $S(\mu') \subset S(\mu)$. Lemma 10 shows us this is not possible. So μ is admissible.

Case 2, $I(\mu) = \frac{3n+k-1}{2}$ and $S(\mu)$ has n points in $(a,\xi]$. It can be observed without too much trouble that there is a non-trivial polynomial P(x) in $(x-\xi)_+^{n-k}, \ldots, (x-\xi)_+^{2n-1}$ with double 0's at each point of $S(\mu)$ in (ξ,b) , with a single 0 at b if $b \in S(\mu)$, and with no other 0's in (ξ,∞) . If $\mu' \geq \mu$,

 $\int P(x) \ d\mu' = \int P(x) d\mu = 0, \text{ by Theorem 3.} \quad \text{If } S_+(\mu) \text{ and } S_+(\mu') \text{ are respectively the points of } S(\mu) \text{ and } S(\mu') \text{ that are greater than } \xi, \text{ we must have } S_+(\mu') \subset S_+(\mu). \text{ Let } \overline{\theta}_+ \text{ and } \overline{\theta}_+' \text{ be respectively the } \mu \text{ and the } \mu' \text{ vectors of weights for the points of } S_+(\mu) \text{ considered as ordered from } \xi \text{ to b. Let } \overline{g}_+(x) = ((x-\xi)_+^{n-k}, \dots, (x-\xi)_+^{2n-1})^T \text{ and let } M_+ \text{ be the matrix with columns } \overline{g}(t_1), \text{ where } t_1 \text{ is the ith element of } S_+(\mu). \text{ The columns of } M_+ \text{ are independent and thus the relationship necessary for } \mu' \geq \mu, \text{ that } M_+ \overline{\theta}_+ = M_+ \overline{\theta}_+', \text{ implies } \overline{\theta}_+ = \overline{\theta}_+' \text{ or that } \mu = \mu' \text{ on } (\xi,b]. \text{ Thus the only way } \mu' \text{ can dominate } \mu \text{ is if } \int_{[a,\xi]}^{-1} \overline{f}(x) \ \overline{f}^T(x) \ d\mu' \geq \int_{[a,\xi]}^{-1} \overline{f}(x) \ \overline{f}^T(x) \ d\mu.$

But this can't happen because by Theorem 2, since $I(\mu) < \infty$, μ is admissible relative to 1,x,..., x^n on [a, ξ]. So μ is admissible.

Case 3, $I(\mu) = \frac{3n+k-1}{2}$ and μ has n points in $[\xi,b)$. We use reasoning parallel to that of case 2, showing any dominating measure must agree with μ on $[a,\xi)$ and noting that μ is admissible with respect to the regular polynomial regression vector on $[\xi,b]$.

The proof is completed by noting that if $I(\mu)$ is smaller than $\frac{3n+k-1}{2}$, $S(\mu)$ is a subspectrum of some admissible spectrum $S(\mu_0)$, where $I(\mu_0) = \frac{3n+k-1}{2}$. Thus by Lemma 2, μ is admissible.

Theorem 6. If $I(\mu) \ge \frac{3n+k+2}{2}$ then μ is inadmissible.

Proof: By Theorem 4 we need only prove this in the case when $I(\mu)$ is finite or when $S(\mu)$ has no more than n-1 points in (a,ξ) or (ξ,b) . We show μ is inadmissible if $I(\mu)=\frac{3n+k+2}{2}$. It will follow from Lemma 2 that μ is inadmissible if $I(\mu)>\frac{3n+k+2}{2}$.

Let \mathcal{M}_{3n+k+2} be the moment space of the functions $1,x,\ldots,x^{2n}$, $(x-\xi)_+^{n-k}$,..., $(x-\xi)_+^{2n}$. That is, \mathcal{M}_{3n+k+2} is the set of all (3n+k+2) vectors

where $\overline{c}=\int\overline{g}(x)\ d\nu$ for $\overline{g}(x)=(1,x,\ldots,x^{2n},(x-\xi)^{n-k}_+,\ldots,(x-\xi)^{2n}_+)^T$ and for ν a finite measure on [a,b]. Then \mathcal{H}_{3n+k+2} is a convex cone in \mathbb{E}^{3n+k+2} . It can be seen from Theorem 3 that if μ is admissible, $\int\overline{g}(x)d\mu$ is a boundary point of \mathcal{H}_{3n+k+2} . This means there is a non-trivial $\overline{\alpha}$ such that $(\overline{\alpha},\int\overline{g}(x)d\mu)=0$ and $(\overline{\alpha},\int\overline{g}(x)d\nu)\leq0$ for all $\nu\neq\mu$. This implies that $P(x)=(\overline{\alpha},\overline{g}(x))$ is a non-trivial polynomial with 0's on $S(\mu)$ and that $P(x)\leq0$ off $S(\mu)$.

Case 1, that $S(\mu)$ does not have n+l points in [a,§] or [§,b]. Then with s=2n and $\ell=n+k$, Lemma 9 tells us there is no non-trivial polynomial with double 0's at the points of $S(\mu)$ interior to [a,b] and with single 0's at a or b if they are in $S(\mu)$. Thus μ is inadmissible.

Case 2, that $S(\mu)$ has n+l points in $[a,\xi]$. Then it is immediate that the first 2n+l coefficients of $\overline{\alpha}$ must be 0 or that P(x) is a polynomial in $(x-\xi)_+^{n-k}, \ldots, (x-\xi)_+^{2n}$. But for this polynomial to have the described property of being 0 on $S(\mu)$ and non-positive off $S(\mu)$, it must have (n+k+l) 0's in $(\xi,b]$. The only way this can happen is if P(x) is also the trivial polynomial in $(x-\xi)_+^{n-k}, \ldots, (x-\xi)_+^{2n}$. So again μ is inadmissible.

Case 3, that $S(\mu)$ has n+l points in [5,b]. This is covered by arguments parallel to those of case 2.

5. Characterization of Admissible Designs, One Knot

From Theorems 5 and 6 we see that the only designs not yet classified are those whose index is $\frac{3n+k}{2}$ or $\frac{3n+k+1}{2}$. These will be handled in this section, by independent arguments.

Definition 7. Let $\mathscr{J}=\{f_1(x),\ldots,f_r(x)\}$ where each $f_1(x)$ is a continuous function on [a,b]. Let $a\leq t_1<\ldots< t_r\leq b$, $\overline{t}=(t_1,\ldots,t_r)^T$, and let $\overline{f}(x)=(f_1(x),\ldots,f_r(x))^T$. Then \mathscr{J} is called a Tchebycheff system or T-system if for all such \overline{t} , det $M(\overline{f},\overline{t})$ has a constant strictly positive or strictly negative sign. \mathscr{J} is called a Weak Tchebycheff system or WT-system if the functions of \mathscr{J} are linearly independent and if for all such \overline{t} , det $M(\overline{f},\overline{t})$ is either always non-negative or always non-positive.

<u>Lemma 11.</u> The system of functions $\{1,x,\ldots,x^S,(x-\xi)_+^{S-\ell},\ldots,(x-\xi)_+^S\}$, $0 \le \ell < s$, is a WT-system on [a,b].

Proof: From relation (3) of Lemma 8 we observe

$$\det M^{T}(\overline{f},\overline{t}) = D(s,\overline{t},\overline{x}) \det M_{1} \det M_{2}$$

and thus that det $M(\overline{f}, \overline{t})$ has a constant sign, since $D(s, \overline{t}, \overline{x}) \ge 0$.

The next lemma gives the existence of a measure μ^* which we will later show dominates μ in the cases considered.

Lemma 12.

- (1) Let n+k be even and $I(\mu) = \frac{3n+k}{2}$. Then if $S(\mu) \subset (a,b)$, there is a μ' with $S(\mu') \not \subset S(\mu)$ such that if $\overline{g}_1(x) = (1,x,\dots,x^{2n-1},(x-\xi)^{n-k}_+,\dots,(x-\xi)^{2n-1}_+)^T$ and $\overline{g}_2(x) = (1,x,\dots,x^{2n-1},(x-\xi)^{n-k}_-,\dots,(x-\xi)^{2n-1}_-)^T$, then $[\overline{g}_1(x) \ d(\mu'-\mu) = 0, \ i=1,2.$
- (2) Let n+k be odd and $I(\mu) = \frac{3n+k+1}{2}$. Then if $S(\mu) \subset (a,b)$, there is a μ' with $S(\mu') \not \subset S(\mu)$ such that if $\overline{g}_1(x) = (1,x,\dots,x^{2n-1})$, $(x-\xi)_+^{n-k-1},\dots,(x-\xi)_+^{2n-1})^T \text{ and } \overline{g}_2(x) = (1,x,\dots,x^{2n-1},(x-\xi)_-^{n-k-1},\dots,(x-\xi)_-^{2n-1})^T,$ then $\int \overline{g}_1(x) \ d(\mu'-\mu) = 0$, i=1,2.

(1966b, pp. 138-9). Let n+k be even, $I(\mu) = \frac{3n+k}{2}$, and $S(\mu) \subset (a,b)$. Let $u_1(x), \dots, u_{3n+k}(x)$ be respectively $1, x, \dots, x^{2n-1}, (x-\xi)^{n-k}_+, \dots, (x-\xi)^{2n-1}_+$. By Lemma 11, $\{u_1(x)\}$ is a WT-system on [a,b]. Let $v_1(t,\delta) = \int_{a-\xi}^{b+\xi} G_{\delta}(x,t)u_1(x)dx$, $i=1,\dots,3n+k$, where $G_{\delta}(x,t) = \frac{1}{\sqrt{2\pi\delta}} \exp[-1/2(\frac{x-t}{\delta})^2]$. Then for fixed $\delta > 0$ it is known that $\{v_1(t,\delta)\}$ is a T-system and that $v_1(t,\delta) \rightarrow u_1(t)$ uniformly on [a,b] as $\delta \downarrow 0$. Let $c_1 = \int u_1(x)d\mu(x)$ and $c_1(\delta) = \int v_1(t,\delta)d\mu(t)$, $i=1,\dots,3n+k$. Then $c_1(\delta) \rightarrow c_1$. Since $\{v_1(t,\delta)\}$ is a T-system, Theorem 2.1 and Corollary 3.1 of Karlin and Studden (1966b, Chap. 2) tell us there is a measure $\overline{\mu}_{\delta}$ with positive mass precisely at a,b and $\frac{3n+k-2}{2}$ points of (a,b) such that $c_1(\delta) = \int v_1(t,\delta)d\overline{\mu}_{\delta}(t)$, $i=1,\dots,3n+k$. Let μ' be a weak limit of $\{\overline{\mu}_{\delta}\}$ with mass on precisely $\leq \frac{3n+k-2}{2}$ points of (a,b). Then $\mu' \not= \mu$ since μ has mass on $\frac{3n+k}{2}$ points of (a,b). Also $c_1 = \int u_1(x)d\mu = \int u_1(x)d\mu'$. By Lemma 10, $S(\mu') \not= S(\mu)$. It is easy to see that $|\overline{\xi}_1(x)d(\mu'-\mu)| = 0$ implies $|\overline{\xi}_2(x)d(\mu'-\mu)| = 0$.

Proof: We proceed along the lines of the proof in Karlin and Studden

The proof for the second part of the lemma is essentially the same and omitted.

Because polynomial spline functions are not infinitely differentiable it is necessary to make a special definition for the multiplicity of a 0.

<u>Definition 8.</u> Let P(x) be a polynomial in the functions $1, x, ..., x^r$, $(x-\xi)_+^{r-\ell}, ..., (x-\xi)_+^{r+1}$, where $r \ge 1$ and $0 \le \ell < r$. Assume P(x) is not identically 0 on any interval and that

$$P^{(0)}(\xi) = P^{(1)}(\xi_{+}) = P^{(1)}(\xi_{-}) = \dots = P^{(k)}(\xi_{+}) = P^{(k)}(\xi_{-}) = 0 \text{ and } P^{(k+1)}(\xi_{-}) \neq P^{(k+1)}(\xi_{+}).$$

(1) If $P^{(k+1)}(x)$ is bounded away from 0 in some neighborhood of ξ and doesn't change sign at ξ , we say P(x) has a 0 of order k+l at ξ .

- (2) If $P^{(k+1)}(x)$ changes sign at ξ , we say P(x) has a O of order k+2 at ξ .
- (3) If $P^{(k+1)}(\xi_+)=0$ or $P^{(k+1)}(\xi_-)=0$ and if $P^{(k+1)}(x)$ does not change sign at ξ , we say P(x) has a 0 of order k+3 at ξ . Multiplicity of a 0 at points other than ξ is defined as usual.

Lemma 13. Let P(x) be a polynomial in the functions $1,x,...,x^r$, $(x-\xi)_+^{r-\ell},...,(x-\xi)_+^{r+l}$, $r \ge 1$ and $0 \le \ell < r$, which is not identically 0 in any interval. Then

- (1) P(x) can have at most (r+l+2) 0's.
- (2) If P(x) has an even order 0 at a point, then P(x) does not change sign at that point.

Proof: We start the proof of part (1) by showing the result true for all r and $\ell=r-1$. P(x) restricted to $[\xi,\infty)$ is a regular polynomial $P_+(x)$ and P(x) restricted to $(-\infty,\xi]$ is the regular polynomial $P_-(x)$. If there are no 0's at ξ , the result is evident because $P_-(x)$ can have at most (r) 0's and $P_+(x)$ at most r+1 for a total of 2r+1=r+(r-1)+2. If there is a 0 of order $h \ge 1$ at ξ , one can observe that the polynomials $P_+(x)$ and $P_-(x)$ can not have more than a total of (r+(r-1)+2-h) 0's in (ξ,∞) and $(-\infty,\xi)$, for a total maximum possible number of r+(r-1)+2. Let us assume the first part of the lemma true for all r and $\ell=r-1,\ldots,r-j+1$, $1< j \le r$. We show it true for $\ell=r-j$. Assume P(x) has more than (2r-j+2) 0's. Then by Rolles Theorem P'(x) has more than (2r-j+1) 0's. This follows since Definition 8 tells us P(x) has a 0 of order i at ξ if and only if P'(x) has a 0 of order i-1 at ξ . But that P'(x) has more than (2r-j+1) 0's contradicts the induction hypothesis since P'(x) is a polynomial in

 $1,x,...,x^{r-1}$, $(x-\xi)_{+}^{(r-1)-(r-j)},...,(x-\xi_{+})^{r}$ and can have at most (r-1)+(r-j)+2=(2r-j+1) O's.

For part (2) we observe from Definition 8 that if P(x) has an even order 0 at ξ and h is the first integer such that $P^{(h+1)}(\xi_-)$ and $P^{(h+1)}(\xi_+)$ are not both 0, then h is even if and only if $P^{(h+1)}(x)$ changes sign at ξ . Noting that the Taylor Formula expression for P(x) is $\frac{P^{(h+1)}(x_1)(x-\xi)^{h+1}}{(n+1)!}$, where x_1 is between ξ and x, we see that P(x) does not change sign at ξ if the order of the 0 at ξ is even. If P(x) has an even order 0 at a point other than ξ it is well known that P(x) does not change sign at the point.

The next lemma exhibits the existence of certain polynomials instrumental in showing which designs are inadmissible.

Lemma 14.

- (1) Let n+k be even, $I(\mu) = \frac{3n+k}{2}$ and $S(\mu) \subset (a,b)$. Then there is a $P_+(x)$ in $1,x,\ldots,x^{2n-1},(x-\xi)^{n-k}_+,\ldots,(x-\xi)^{2n}_+$ such that the coefficient of $(x-\xi)^{2n}_+ > 0$, $P_+(x) = 0$ on $S(\mu)$, $P_+(x) \geq 0$ on [a,b], and $P_+(x) > 0$ on the points of $[\xi,b]$ not in $S(\mu)$. There is a $P_-(x)$ in $1,x,\ldots,x^{2n-1}$, $(x-\xi)^{n-k}_-,\ldots,(x-\xi)^{2n}_-$ such that the coefficient of $(x-\xi)^{2n}_- > 0$, $P_-(x) = 0$ on $S(\mu)$, $P_-(x) \geq 0$ on [a,b], and $P_-(x) > 0$ on the points of $[a,\xi]$ not in $S(\mu)$.
- (2) Let n+k be odd, $I(\mu) = \frac{3n+k+1}{2}$ and $S(\mu) \subset (a,b)$. Then there is a $P_{+}(x)$ in $1,x,\ldots,x^{2n-1},(x-\xi)^{n-k-1}_{+},\ldots,(x-\xi)^{2n}_{+}$ such that the coefficient of $(x-\xi)^{2n}_{+} > 0$, $P_{+}(x) = 0$ on $S(\mu)$, $P_{+}(x) \geq 0$ on [a,b], and $P_{+}(x) > 0$ on the points of $[\xi,b]$ not in $S(\mu)$. There is a $P_{-}(x)$ in $1,x,\ldots,x^{2n-1},(x-\xi)^{n-k-1}_{-},\ldots,(x-\xi)^{2n}_{-}$ such that the coefficient of

 $(x-\xi)^{2n}_->0$, $P_-(x)=0$ on $S(\mu)$, $P_-(x)\geq 0$ on [a,b], and $P_-(x)>0$ on the points of $[a,\xi]$ not in $S(\mu)$.

Proof: We merely establish the existence of $P_{+}(x)$ for the first part. The existence of the other polynomials follows from similar arguments.

Case 1, that there are n points of $S(\mu)$ in $(a,\xi]$. Let $\overline{f}(x) = (1,x,\ldots,x^{2n-1},(x-\xi)^{n-k}_+,\ldots,(x-\xi)^{2n-1}_+)^T \text{ and let } r_1,\ldots,r_{\underline{3n+k}}$ be the

points of $S(\mu)$ ordered from left to right. Let $t_1 = t_2 = r_1, \dots, t_{3n+k-1} = t_{3n+k} = r_{3n+k}$. By Lemma 8, $M(\overline{f}, \overline{t})$ is non-singular. Thus there is an $\overline{\alpha}$

such that

$$M^{T}(\overline{f}, \overline{t}) \ \overline{\alpha} = (0, \dots, 0, -(r_{\underline{2n+1}} - \xi)^{2n}, -2n(r_{\underline{2n+1}} - \xi)^{2n-1}, \dots, -(r_{\underline{3n+k}} - \xi)^{2n},$$

$$-2n(r_{\underline{3n+k}} - \xi)^{2n-1})^{T}.$$

Let $M_2^T(\overline{f},\overline{t})$ be the matrix consisting of the last n+k columns of $M^T(\overline{f},\overline{t})$. It can be seen that the first 2n rows of $M_2^T(\overline{f},\overline{t})$ are 0 and that the lower right (n+k)x(n+k) submatrix is non-singular. Thus $\overline{\alpha}$ has its first 2n components 0. Then $P_+(x) = (\overline{\alpha},\overline{f}(x))+(x-\xi)_+^{2n}$ is a non-trivial polynomial in $(x-\xi)_+^{n-k},\ldots,(x-\xi)_+^{2n}$ with (n+k) 0's in (ξ,b) . Since $P_+(x)$ can't have any other 0's in (ξ,∞) , since $P_+(x)$ $+\infty$ as $x\to\infty$, and since $P_+(x)=0$ for $x\leq \xi$, it is clear that $P_+(x)$ satisfies the conditions of the lemma.

Case 2, that there are fewer than n points of $S(\mu)$ in $(a,\xi]$. Again $M(\overline{f},\overline{t})$ is non-singular. If $\overline{\alpha}$ is the solution to

$$M^{T}(\overline{f}, \overline{t})\overline{\alpha} = (-(r_{1} - \xi)_{+}^{2n}, -2n(r_{1} - \xi)_{+}^{2n-1}, \dots, -(r_{\underline{3n+k}} - \xi)_{+}^{2n}, -2n(r_{\underline{3n+k}} - \xi)_{+}^{2n-1})^{T},$$

 $P_+(x)=(\overline{f}(x),\overline{\alpha})+(x-\xi)_+^{2n}$ is the polynomial we seek. We note that if $P_+(x)$ were identically 0 on $[a,\xi]$, it would be a polynomial in $(x-\xi)_+^{n-k}$,..., $(x-\xi)_+^{2n}$ having more than (n+k) 0's on (ξ,b) and thus trivial there too. So $P_+(x)$ is non-trivial on $[a,\xi]$ and on $[\xi,b]$. From Lemma 13, with r=2n-1 and $\ell=n+k-1$, we get $P_+(x)$ can have at most (3n+k) 0's. But $P_+(x)$ is defined so that it has a double 0 at each of the $\frac{3n+k}{2}$ points of $S(\mu)$. Since $P_+(x) \to \infty$ as $x \to \infty$ and since, also by Lemma 13, $P_+(x)$ can't change sign, $P_+(x) \ge 0$ for all x and satisfies the conditions of the lemma.

The next theorem classifies some of the spectra of indices $\frac{3n+k}{2}$ and $\frac{3n+k+1}{2}$ as inadmissible.

Theorem 7.

- (1) If n+k is even, a measure μ of index $\frac{3n+k}{2}$ is inadmissible if $S(\mu)$ doesn't include a and b.
- (2) If n+k is odd, a measure μ of index $\frac{3n+k+1}{2}$ is inadmissible if $S(\mu)$ doesn't include a and b.

(Note that the indices in parts (1) and (2) are integers, so that either both or none of a and b are in $S(\mu)$.)

Proof:

(1) Consider the $\mu^{\,\prime}\,$ from Lemma 12, part (1). Consider the $P_+(x)$ and $P_-(x)\,$ from Lemma 14, part (1) and write

$$P_{+}(x) = (x-\xi)_{+}^{2n} + \overline{P}_{+}(x)$$

$$P_{x}(x) = (x-\xi)^{2n} + \overline{P}_{x}(x)$$

where $\overline{P}_{+}(x)$ is a polynomial in the functions $1,x,\ldots,x^{2n-1},(x-\xi)^{n-k}_{+},\ldots,(x-\xi)^{2n-1}_{+}$. The measure μ' satisfies $\int \overline{P}_{+}(x)d\mu' = \int P_{+}(x)d\mu$. We notice $\int P_{+}(x)d\mu=0$, $\int P_{+}(x)d\mu' \geq 0$ and $\int P_{+}(x)d\mu' > 0$ if $S(\mu')$ has a point in $[\xi,b]$ not in $S(\mu)$, and that $\int P_{-}(x)d\mu' \geq 0$ and $\int P_{-}(x)d\mu' > 0$ if $S(\mu')$ has a point in $[a,\xi]$ not in $S(\mu)$. Thus $\int (x-\xi)^{2n}_{+}d(\mu'-\mu) \geq 0$, $\int (x-\xi)^{2n}_{-}d(\mu'-\mu) \geq 0$ and at least one inequality is strict. By Theorem 3', $\mu' \geq \mu$.

(2) Here we use the μ ' of Lemma 12, part (2) to dominate μ . We show μ ' $\geq \mu$ as we did in part (1), using $P_{+}(x)$ and $P_{-}(x)$ from Lemma 14, part (2).

Corollary. If n+k is even, a measure of index $\geq \frac{3n+k+1}{2}$ is inadmissible.

Proof: This follows because the spectrum of such a measure is the superspectrum of a measure of index $\frac{3n+k}{2}$ whose spectrum is contained in (a,b).

The only remaining unclassified designs are those of indices $\frac{3n+k}{2}$ and $\frac{3n+k+1}{2}$ that are not covered in the above theorem or corollary. The next theorem shows them admissible.

Theorem 8.

- (1) If n+k is even, a measure μ of index $\frac{3n+k}{2}$ is admissible if $S(\mu)$ contains a and b.
- (2) If n+k is odd, a measure μ of index $\frac{3n+k+1}{2}$ is admissible if $S(\mu)$ contains a and b.

Proof:

(1) Case 1, that there are not n points of $S(\mu)$ in either $(a,\xi]$ or $[\xi,b)$. Assume μ is inadmissible. By Lemma 3, there is an admissible $\mu' \geq \mu$. By Theorem 7, $S(\mu')$ can have at most $\frac{3n+k}{2}-1$ points in (a,b).

Case 2, that there are n points of $S(\mu)$ in $(a,\xi]$. Then the points of $S(\mu)$ to the right of ξ are b and $\frac{n+k-2}{2}$ points of (ξ,b) . Assume $\mu' \geq \mu$. First we show that μ' must agree with μ on $(\xi,b]$. Notice that there is a polynomial P(x) in the functions $(x-\xi)^{n-k}_+, \dots, (x-\xi)^{2n-1}_+$ with a single 0 at b, a double 0 at each point of $S(\mu)$ in (ξ,b) and no other 0's in $(\xi,b]$. Since $\int P(x) d(\mu'-\mu) = 0$ there is no point p in $(\xi,b]$ that is in $S(\mu')$ and not in $S(\mu)$. Arguing as we did in the proof of Theorem 5, we get $\mu' = \mu$ on $(\xi,b]$ and also, since μ is admissible with respect to the regular polynomial regression vector on $[a,\xi]$, that $\mu' = \mu$ on $[a,\xi]$. Thus there is no $\mu' > \mu$.

Case 3, that there are n points of $S(\mu)$ in [5,b) follows from symmetric arguments.

(2) Case 1, that $S(\mu)$ does not have n points in $(a,\xi]$ or in $[\xi,b)$. Assume an admissible μ' dominates μ . Then μ' can have at most $\frac{3n+k-1}{2}$ points in (a,b). Let $r_1,\ldots,r_{\frac{3n+k-1}{2}}$ be the points of $S(\mu)$ in

(a,b). We now show that $S(\mu')$ must have a point in each of the open intervals (r_i, r_{i+1}) , $i = 1, ..., \frac{3n+k-3}{2}$. For assume not; assume that there is no point of $S(\mu')$ in (r_i, r_{i+1}) . Then by Lemma 9 there is a polynomial P(x)in the components of $\overline{g}(x) = (1,x,\ldots,x^{2n-1},(x-\xi)^{n-k}_+,\ldots,(x-\xi)^{2n-1}_+)^T$ with single 0's at a,b, r_i , r_{i+1} , double 0's at the other points of $S(\mu)$ in (a,b), and no other 0's. Then as in the first case of part 1, $\int P(x) d(\mu' - \mu) \neq 0$ and $\mu' \ngeq \mu$. We can thus assume that either (a,r_1) or $(r_{\underline{3n+k-1}}$,b) does not contain a point of $S(\mu^{\,\imath})$. Without loss of generality we assume there is no point of $S(\mu')$ in (a,r_1) . Let $\overline{t} = (t_1,...,t_{3n+k})^T$ where $t_1 = a$, $t_2 = r_1, t_3 = t_4 = r_2, \dots, t_{3n+k} = b.$ Let $\overline{h}(\overline{t}) = ((t_1 - \xi)_+^{2n}, (t_2 - \xi)_+^{2n}, (t_3 - \xi)_+^{2n},$ $2n(t_{4}-\xi)_{+}^{2n-1},\dots,(t_{3n+k-2}-\xi)_{+}^{2n},\ 2n(t_{3n+k-1}-\xi)_{+}^{2n-1},\ (t_{3n+k}-\xi)_{+}^{2n})^{T}.\quad \text{By Lemma}$ 8, $M(\overline{g}, \overline{t})$ is non-singular. Let $\overline{\alpha}$ be the solution of $M^{T}(\overline{g}, \overline{t})\overline{\alpha} = -\overline{h}(\overline{t})$. Let $P(x) = (x-\xi)_+^{2n} + (\overline{g}(x), \overline{\alpha})$. Then P(x) has a 0 at each of the t_i and can't have any other 0's, by Lemma 13. Also $P(x) \le 0$ for all points of $S(\mu')$, P(x) < 0 for some points of $S(\mu')$, and P(x) = 0 on $S(\mu)$. Thus we get $\int (x-\xi)_+^{2n} d(\mu'-\mu) < 0$. So μ is admissible, because this last inequality contradicts $\mu' \ge \mu$, by Theorem 3.

Case 2, that $S(\mu)$ has n points in $(a,\xi]$ and thus b and $\frac{n+k-1}{2}$ points of $S(\mu)$ in $(\xi,b]$. Assume $\mu' \geq \mu$. Theorem 1.1 of Karlin and Studden (1966b, Chap. 3) tells us that if $\overline{g}(x) = ((x-\xi)_+^{n-k}, \dots, (x-\xi)_+^{2n-1})^T$, then subject to $\overline{g}(x)$ d $(\nu-\mu) = 0$, $\int (x-\nu)_+^{2n} d\nu$ is uniquely maximized for ν on $(\xi,b]$ by $\nu = \mu$ and thus, by Theorem 3, that $\mu' = \mu$ on $(\xi,b]$. We proceed as before from this point, case 3 following from symmetric arguments.

Corollary. If n+k is odd, a measure of index $\leq \frac{3n+k}{2}$ is admissible. Proof: We merely note that the spectrum of such a measure is the subspectrum of an admissible spectrum of index $\frac{3n+k+1}{2}$.

From Theorems 7 and 8 we get that if n+k is even, then designs of index $<\frac{3n+k}{2}$ are admissible, that designs of index $\frac{3n+k}{2}$ are admissible if and only if they contain a and b, and that designs of index $>\frac{3n+k}{2}$ are inadmissible. We get that if n+k is odd, then designs of index $<\frac{3n+k+1}{2}$ are admissible, that designs of index $\frac{3n+k+1}{2}$ are admissible if and only if they contain a and b, and that designs of index $>\frac{3n+k+1}{2}$ are inadmissible. We put these facts together in the final theorem of the chapter.

Theorem 9. Relative to $f(x) = (1, x, ..., x^n, (x-\xi)_+^{n-k}, ..., (x-\xi)_+^n)^T$ (or $\overline{f}(x) = (1, x, ..., x^n, (x-\xi)_-^{n-k}, ..., (x-\xi)_-^n)^T$) μ is admissible if and only if

- (1) $S(\mu)$ has no more than n-l points in either (a, ξ) or (ξ , b) and
- (2) $S(\mu)$ has fewer than $n + \frac{n+k}{2}$ points in (a,b).

CHAPTER II

THE CASE OF MORE THAN ONE KNOT

1. Necessary and Sufficient Moment Conditions

Now we are concerned with the case of h knots, i.e., the case where the regression vector $\overline{f}(x) = (1,x,\ldots,x^n, (x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^n,\ldots,(x-\xi_1)_+^$

Lemma 15. Let M be a square matrix of the form

$$\begin{pmatrix} A_1 & A_2 & \cdots & A_{\ell} \\ A_2 & A_2 & \cdots & A_{\ell} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ A_{\ell} & A_{\ell} & \cdots & A_{\ell} \end{pmatrix}.$$

Then $M \ge 0$ if and only if $0 \neq A_1 \ge \cdots \ge A_\ell \ge 0$.

Proof: We need only notice that

$$(x_1,...,x_l) M (x_1,...,x_l)^{T_n} \sum_{i=1}^{l} (A_i - A_{i+1}) (x_1 + ... + x_i)^2$$

where $A_{\ell+1} \equiv 0$. Then for $x_2 = x_3 = ... = x_{\ell} = 0$, $(A_1 - A_2)x_1^2 \ge 0$ for all

 $x_1 \Leftrightarrow A_1 \geq A_2$. For $x_3 = x_4 = \dots = x_\ell = 0$, $(A_1 - A_2)x_1^2 + (A_2 - A_3)(x_1 + x_2)^2 \geq 0$ for all x_1 and $x_2 \Leftrightarrow A_1 \geq A_2 \geq A_3$. Proceeding in this way we arrive at $\overline{x} \to \overline{x} \to 0$ for all $\overline{x} \Leftrightarrow A_1 \geq A_2 \geq \dots \geq A_\ell \geq A_{\ell+1} = 0$. Noting that M non-negative definite and $A_1 = 0 \Leftrightarrow M = 0$, we are done.

(2)
$$0 \neq \int x^{2n} d(\mu' - \mu) \geq \int (x - \xi_1)_+^{2n} d(\mu' - \mu) \geq \dots \geq \int (x - \xi_h)_+^{2n} d(\mu' - \mu) \geq 0.$$

Proof: The proof is essentially like that of Theorem 3 and so we only sketch it. Lemma 7 is used to show (1) holds if $M = M(\mu^*) - M(\mu) \ge 0$. Lemma 15 shows that given (1), $M \ge 0$ if and only if (2) holds.

2. Subadmissibility

In Section 4 of Chapter I we showed that if μ is inadmissible on either $[a,\xi]$ or $[\xi,b]$ with respect to the regular polynomial regression vector $\overline{f}(x)=(1,x,\ldots,x^n)^T$ then μ is inadmissible with respect to the spline regression vector $\overline{f}(x)=(1,x,\ldots,x^n,(x-\xi)_+^{n-k},\ldots,(x-\xi)_+^n)^T$. In effect we showed that a design inadmissible with respect to 0 knots was inadmissible with respect to 1 knot. Now we will show that a design inadmissible with respect to ℓ knots is inadmissible with respect to ℓ knots. First we give some definitions.

Definition 9. Let ξ_0 = a and ξ_h +l = b. By an interval of length ℓ , $0 \le \ell \le h$, we mean one of the intervals $[\xi_i, \xi_{i+\ell+1}]$.

Note that an interval of length ℓ is characterized by the fact that it has ℓ knots in its interior.

Definition 10. Let ξ_0 = a and ξ_{h+1} = b. A measure μ that is admissible on all intervals of length ℓ < h, say $\{[\xi_{i_0}, \xi_{i_0}, \xi_{i_0}, \xi_{i_0}]\}$, relative to the regression vectors $\overline{f}(x) = (1, x, \dots, x^n, (x - \xi_{i_0} + 1)^{n-k}, \dots, (x - \xi_{i_0} + 1)^n, \dots, (x - \xi_{i_0} + 1)^n, \dots, (x - \xi_{i_0} + \ell)^n\}$ respectively, is said to be subadmissible (h).

Theorem 11. Let μ be admissible for h knots. Then $\dot{\mu}$ is subadmissible (h).

Proof: Assume that μ is not subadmissible. Then for some i_{0} and some $\ell < h$, μ is inadmissible on $\left[\xi_{i_{0}}, \xi_{i_{0}+\ell+1}\right]$ relative to $\overline{f}(x) = (1,x,\ldots,x^{n},(x-\xi_{i_{0}+1})^{n-k}_{+},\ldots,(x-\xi_{i_{0}+\ell})^{n-k}_{+},\ldots,(x-\xi_{i_{0}+\ell})^{n-k}_{+},\ldots,(x-\xi_{i_{0}+\ell})^{n}_{+})^{T}$. Thus there is a $\hat{\mu}$ on $\left[\xi_{i_{0}}, \xi_{i_{0}+\ell+1}\right]$ such that $\hat{\mu} \geq \mu$ on $\left[\xi_{i_{0}}, \xi_{i_{0}+\ell+1}\right]$ or such that

(1)
$$\int_{[\xi_{i_0}, \xi_{i_0} + \ell + 1]} \overline{g}_0(x) d(\hat{\mu} - \mu) = 0$$
 and

$$(2) \quad 0 \neq \int_{\left[\xi_{i_{0}}, \xi_{i_{0}} + \ell + 1\right]}^{x^{2n}} d(\hat{\mu} - \mu) \geq \int_{\left[\xi_{i_{0}}, \xi_{i_{0}} + \ell + 1\right]}^{(x - \xi_{i_{0}} + \ell + 1)}^{(x - \xi_{i_{0}} + \ell + 1)}^{(x - \xi_{i_{0}} + \ell + 1)} d(\hat{\mu} - \mu)$$

$$\geq \cdots \geq \int_{\left[\xi_{i_{0}}, \xi_{i_{0}} + \ell + 1\right]}^{(x - \xi_{i_{0}} + \ell + 1)}^{(x - \xi_{i_{0}} + \ell + 1)}^{2n} d(\hat{\mu} - \mu) \geq 0,$$

where $\overline{g}_{O}(x) = (1, x, ..., x^{2n-1}, (x-\xi_{i_{O}+1})_{+}^{n-k}, ..., (x-\xi_{i_{O}+1})_{+}^{2n-1}, ..., (x-\xi_{i_{O}+\ell})^{n-k}$ $,..., (x-\xi_{i_{O}+\ell})_{+}^{2n-1})^{T}$. Let μ' be defined as $\hat{\mu}$ on $[\xi_{i_{O}}, \xi_{i_{O}+\ell+1}]$ and μ [a,b]-[ξ_i , ξ_i + ℓ +l]. Then if g(x) is as in Theorem 10, conditions (1) and (2) just above imply

(3)
$$\int_{[a,b]} \overline{g}(x) d(\mu'-\mu) = 0 \text{ and }$$

(4)
$$0 \neq \int_{[a,b]} x^{2n} d(\mu' - \mu) \geq ... \geq \int_{[a,b]} (x - \xi_h)_+^{2n} d(\mu' - \mu),$$

which, by Theorem 10, implies $\mu' \geq \mu$.

3. Some Particular Results

Without too much new theory we are able to classify some subadmissible designs as admissible. Roughly speaking, if a subadmissible design doesn't have too many points in $(\xi_h, b]$ or $[a, \xi_1)$ it will be admissible. Let $\overline{f}(x) = (1, x, \dots, x^n, (x - \xi_1)_+^{n-k}, \dots, (x - \xi_1)_+^n, \dots, (x - \xi_h)_+^{n-k}, \dots, (x - \xi_h)_+^n)^T \quad \text{and} \quad x - \xi_h = (1, x, \dots, x^n, (x - \xi_h)_+^n)^T$ let μ be subadmissible (h), which means, in particular, that μ is admissible on $[a,\xi_h]$. Let $S(\mu)$ have r points in (ξ_h,b) and s points at b (s = 0 or 1). Let $V(\mu) \equiv 2r+s$ and let $\overline{g}_{+}(x) = ((x-\xi_{h})_{+}^{n-k}, \dots, (x-\xi_{h})_{+}^{2n-1})^{T}$. Notice that by Theorem 10, if $\mu' \ge \mu$ then $\int_{\overline{g}_{+}}(x) d(\mu' - \mu) = 0$. Assume $\mu' \geq \mu$. Now if $V(\mu) < n+k$ it follows from Theorem 2.1 of Karlin and Studden (1966b, p. 42) that μ ' agrees with μ on (ξ_h ,b]. This theorem says that if $V(\mu)$ is smaller than the number of functions in a Tchebycheff system whose integrals are to be fixed, then there is no other measure μ ' that fixes the integrals at the same values. If $V(\mu) = n+k$ and n+k is odd (i.e., b \in S(μ)), then by Theorem 1.1 of Karlin and Studden (1966b, p. 80) if $\int \overline{\xi}_{+}(x) d(\mu' - \mu) = 0$, $\int (x - \xi_{h})_{+}^{2n} d(\mu' - \mu) < 0$ unless $\mu' = \mu$ on $(\xi_{h}, b]$. Since the negativity of the last integral contradicts $\mu' \geq \mu$ (by Theorem 10) we get $\,\mu'$ = μ on (ξ_h,b]. Thus in the two cases: $V(\mu)$ < n+k and $V(\mu)$ = n+k

when n+k is odd, we get $\mu=\mu'$ on $(\xi_h,b]$. But since μ is admissible on $[a,\xi_h]$ we must also have $\mu=\mu'$ on $[a,\xi_h]$. Thus $\mu'\geq\mu$ is impossible. We state these results as a theorem, including also the similar case when $S(\mu)$ has a small enough number of points in $[a,\xi_1)$.

Theorem 12. Let μ be subadmissible (h). Let $S(\mu)$ have r_+ points in (ξ_h,b) and s_+ points at b (s_+ = 0 or 1); let $S(\mu)$ have r_- points in (a,ξ_1) and s_- points at a (s_- = 0 or 1). Let $V_+(\mu) = r_+ + s_+$ and let $V_-(\mu) = r_- + s_-$. Let $V(\mu) = \min(V_+(\mu),V_-(\mu))$. Then if $V(\mu) < n+k$ or if n+k is odd and $V(\mu) = n+k$, μ is admissible.

Example 1. Let k be as large as we permit, i.e., k = n-l. We let ξ_0 = a and ξ_{h+1} = b and show that a design is admissible if and only if it has fewer than n points in each of the intervals (ξ_1, ξ_{i+1}) , i = 0,...,h. We observe from Chapter I that this result is true in both the case of 0 knots and the case of one knot. So we assume it is true for h-l knots and show it true for h knots. Let μ be a design with fewer than n points in each open interval. Then by the induction hypothesis it is subadmissible (h). By the theorem it is admissible since n+k is odd. If μ has n or more points in an interval it is clearly not subadmissible (h) and thus not admissible. So we are done.

Notice that when k=n-1 a polynomial in the components of the regression vector is a regular nth degree polynomial on each $[\xi_i, \xi_{i+1}]$ and needs only be continuous at the knots.

In the case when n=1, the above result tells us that μ is admissible if and only if $S(\mu) \subset \{a,\xi_1,\ldots,\xi_h,b\}$.

Example 2. Let n=3, k=0, h=2. Then a design is subadmissible (2) if and only if it has fewer than 3 points in (a,ξ_1) , (ξ_1,ξ_2) , (ξ_2,b) and fewer than 5 points in (a,ξ_2) and (ξ_1,b) . It follows from the theorem that a design that is subadmissible (2) and has a single point in (ξ_2,b) (in (a,ξ_1)) and a single point at b (at a) is admissible. The only designs still undetermined in this case are among those that are subadmissible (2) and have two points in both (a,ξ_1) and (ξ_2,b) .

Example 3. n = 4, k = 0, h = 2. Here the subadmissible (2) designs are those with fewer than 4 points in (a, ξ_1) , (ξ_1, ξ_2) , (ξ_2, b) and fewer than 6 points in (a, ξ_2) and (ξ_1, b) . Notice that any subadmissible (2) design with only one point in (a, ξ_1) or (ξ_2, b) is admissible. The designs undetermined are among those subadmissible (2) designs with more than 1 point in both (a, ξ_1) and (ξ_2, b) .

4. The Case of a Second Differentiable Regression Function

In this section we assume that k = n-2 ($n \ge 2$) and classify many designs for h knots. In other words, we work under the assumption that the regression polynomial has at least a continuous first derivative at the knots. The techniques of this section will be generalizations of techniques used mainly in Section 5 of Chapter I. First we generalize Lemma 8 which was a handy tool throughout most of Chapter I.

Lemma 16. Let $a \le t_1 \le \dots \le t_{s+h\ell+h+1} \le b$ where there are no more than $(s+l-\ell)$ t's at a point ξ_1 and where no more than (s+l) t's coincide anywhere. Then if $\overline{f}(x) = (1,x,\dots,x^s,(x-\xi_1)_+^{s-\ell},\dots,(x-\xi_1)_+^s,\dots,(x-\xi_h)_+^{s-\ell},\dots,(x-\xi_h)_+^s)^T$, $0 \le \ell \le s-l$, $M(\overline{f},\overline{t})$ is non-singular if and only if

(1)
$$t_{r(\ell+1)} < \xi_r$$
 and

(2)
$$\xi_r < t_{s+2+(r-1)(\ell+1)}$$
, $r = 1,...,h$.

Proof: This result follows from the Karlin and Ziegler result mentioned before Lemma 8 in essentially the same way Lemma 8 followed.

We now define a concept which, after an induction later on, will be shown related to subadmissibility (h). We define this concept of ''permissibility'' for the case when n+k is even, but in this section use it only when k=n-2.

Definition 12. Let n+k be even. A design μ is said to be permissible (h) if $S(\mu)$ has at most $\left(n+\frac{\ell}{2}\left(n+k\right)-1\right)$ points in the interior of each interval of length ℓ , for $0 \le \ell < h$. Otherwise μ is said to be non-permissible (h).

Next comes a lemma that generalizes Lemma 14 and leads to the determination of a large class of inadmissible designs.

Lemma 17. Let $n \ge 2$ and k = n-2. Let μ be a permissible (h) design with precisely $n + \frac{h}{2}$ (n+k) points in $S(\mu)$, all in (a,b). Then there exists a set of polynomials $\{P_i(x)\}_{i=0}^h$ where $P_i(x)$ is a polynomial in the components of $\overline{g}(x) = (1,x,\ldots,x^{2n-1},(x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^{2n-1},\ldots,(x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^{2n-1},\ldots,(x-\xi_1)_+^{2n-1},\ldots,(x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^{2n-1})^T$ and $f_i(x)$, where

$$f_{o}(x) = x^{2n} - (x - \xi_{1})_{+}^{2n},$$

$$f_{i}(x) = (x - \xi_{i})_{+}^{2n} - (x - \xi_{i+1})_{+}^{2n}, i = 1,...,h-1, and$$

$$f_{h}(x) = (x - \xi_{h})_{+}^{2n},$$

such that

- (1) The coefficient of $f_i(x) = 1$ and
- (2) $P_i(x) = 0$ on $S(\mu)$, $P_i(x) \ge 0$ everywhere,

and $P_{i}(x) > 0$ on the points of $[\xi_{i}, \xi_{i+1}]$ not in $S(\mu)$.

Proof: It will be observed that a permissible (h) design μ with $S(\mu)$ having precisely $n+\frac{h}{2}$ (n+k) points, all in (a,b), must have (n-l) points in (a, ξ_1) and (ξ_2 ,b), one point at each of the h knots, and (n-2) points in each (ξ_1 , ξ_{1+1}), for $i=1,\ldots,h-1$.

For i=0 or h the result follows immediately as in the proof of Lemma 14, case 1. $P_h(x)$ will be 0 on $[a,\xi_h]$ and $P_o(x)$ will be 0 on $[\xi_1,b]$. For $i=1,\ldots,h-1$, the technique is essentially the same. We show there is a non-negative, non-trivial polynomial in $(x-\xi_i)_+^2,\ldots,(x-\xi_i)_+^{2n-1}$, $(x-\xi_{i+1})^2,\ldots,(x-\xi_{i+1})^{2n-1}$, and $f_i(x)$ with double 0's at the points of $S(\mu)$ in $[\xi_i,\xi_{i+1}]$ that is 0 on the complement of $[\xi_i,\xi_{i+1}]$. Using Lemma 8 as was done in Lemma 14, it is not too hard to see that there is a polynomial P(x) in $1,x,\ldots,x^{2n-1},(x-\xi_{i+1})_+^2,\ldots,(x-\xi_{i+1})_+^{2n-1}$ and $x^{2n}-(x-\xi_{i+1})_+^{2n}$ that has double 0's at the points of $S(\mu)$ in $[\xi_i,\xi_{i+1}]$ and is identically 0 to the right of ξ_{i+1} . P(x) has no other 0's on $[\xi_i,\xi_{i+1}]$ and $P(x) \geq 0$ there if the coefficient of $x^{2n}-(x-\xi_{i+1})_+^{2n}$ is 1. If we let

$$P_{i}(x) = \begin{cases} P(x), & x \geq \xi_{i} \\ 0, & x < \xi_{i} \end{cases}$$

then $P_i(x)$ satisfies the conditions of the lemma. Next we generalize Lemmas 10 and 12.

Proof: The proof of this follows from Lemma 16 in the same way the proof of Lemma 10 followed from Lemma 8.

Lemma 19. Let n+k be even and let $S(\mu)$ have precisely $n+\frac{h}{2}$ (n+k) points, all in (a,b). Then if $\overline{g}(x)=(1,x,\ldots,x^{2n-1},(x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^{2n-1})^T$, there is a μ' such that $|\overline{g}(x)| d(\mu'-\mu)=0$ and $S(\mu') \not = S(\mu)$.

Proof: The proof of this is essentially the same as the proof of Lemma 12, using the fact that the component functions of $\overline{\mathbf{g}}(\mathbf{x})$ constitute a WT-system and using Lemma 18 where Lemma 12 used Lemma 10.

We are now in a position to give a generalization of Theorem 7, showing certain designs besides those not subadmissible (h) are inadmissible.

Theorem 13. Let $n \ge 2$ and k = n-2. Then a design μ such that $S(\mu)$ has precisely $n + \frac{h}{2}(n+k) = n+h(n-1)$ points, all in (a,b), is inadmissible.

Proof: We show this result by induction. First note that it is true in the polynomial case (0 knots) and also in the case of 1 knot. So assume it is true for 1,...,h-1 knots. If this be the case, a non-permissible (h) design is not subadmissible (h) and so we need only consider permissible (h) designs. Let $\overline{g}(x) = (1,x,\ldots,x^{2n-1},(x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^{2n-1},\ldots,(x-\xi_h)_+^{n-k},\ldots$

satisfied and thus $\mu' \geq \mu$.

Corollary 1. If μ is non-permissible (h), then μ is not subadmissible (h).

Corollary 2. If $S(\mu)$ has n+h(n-1) or more points in (a,b), then μ is inadmissible.

Using Theorem 12 we see that the admissible designs must lie in the class of designs that are permissible (h). In addition we can say that an admissible design can have at most $(\ell+1)(n-1)$ points in any interval of length ℓ , for $\ell \leq h$. We are able to classify many designs with these properties as admissible.

Theorem 14. Let $n \geq 2$, k = n-2, and μ be a permissible (h) design with points of $S(\mu)$ at a, b and at precisely (h+l)(n-l) points of (a,b), none of which is a knot ξ_i , $i = 1, \ldots, h$. Then μ is admissible.

Proof: Note that the condition of permissibility (h) and the fact that $S(\mu)$ misses the knots imply that $S(\mu)$ has precisely n-1 points in each open interval, (ξ_1, ξ_{i+1}) , $i=0,\ldots,h$. Assume $\mu' \geq \mu$, where μ' is permissible (h). Also assume the result is true for fewer than h knots. Thus without loss of generality we can assume $\mu' \not= \mu$ on $(\xi_h, b]$, for then μ' would have to dominate μ on $[a, \xi_h]$, which by the induction hypothesis is impossible. Let $\overline{g}_+(x) = ((x-\xi_h)_+^2, \ldots, (x-\xi_h)_+^{2n-1})^T$. It follows from Theorem 1.1 of Karlin and Studden (1966b, p.80) that μ' can't have all of its mass points in $(\xi_h, b]$ concentrated in the subinterval $[\beta_1, b]$, where β_1 is the first mass point of μ in $(\xi_h, b]$, because of all measures ν on $[\beta_1, b]$ such that $\int \overline{g}_+(x) \ d(\nu-\mu) = 0$, μ uniquely maximizes $\int (x-\xi_h)_+^{2n} \ d\nu$. It follows from Theorem 2.1 of Karlin and Studden (1966b, p.42) that μ'

must have at least n-l points in (ξ_h,b) and, since μ' is permissible, it follows that μ' must have precisely n-l points in (ξ_h,b) . Lemma 3.1 of Karlin and Studden (1966b, p.47) tells us that the mass points of μ and μ' are interwoven, or in particular that there is no mass point of μ' between the last point of $S(\mu)$ in (ξ_h,b) and b. Define the vector $\overline{t}=(t_1,\ldots,t_{2n+2h(n-1)})^T$ as follows: Let $t_1=t_2=a$, $t_3=t_4=the$ first point of $S(\mu)$ in $(a,b),\ldots$, $(2\ t_i$'s for each point of $S(\mu)$ in (a,b) up to and including the next to last one), $t_{2n+2h(n-1)-1}=the$ last point of $S(\mu)$ in (a,b), and $t_{2n+2h(n-1)}=b$. Then

$$\begin{array}{lll} t_{2n-2} & <\xi_1, & & \xi_1 < t_{2n+1}, \\ t_{4n-4} & <\xi_2, & & \xi_2 < t_{2n+1+(2n-2)}, \\ & \vdots & & \vdots & & \vdots \\ t_{2h(n-1)} & <\xi_h, & & \xi_h < t_{2n+1+(h-1)(2n-2)}. \end{array}$$

Let $\overline{g}(x) = (1,x,\ldots,x^{2n-1},(x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^{2n-1},\ldots,(x-\xi_h)_+^{n-k},\ldots,(x-\xi_h)_+^{n-k})^T$. Then by Lemma 16, $M(\overline{g},\overline{t})$ is non-singular. Let $\overline{\alpha}$ be the solution to $M^T(\overline{g},\overline{t})$ $\overline{\alpha} = (0,1,0,\ldots,0)^T$ and let $P(x) = (\overline{g},(x),\overline{\alpha})$. Then P(x) has a single 0 at a, b, and the last point of $S(\mu)$ in (a,b) and P'(a) = 1. We now show P(x) is not 0 anywhere else on [a,b]. Assume P(x) has another 0 point at t_0 . Let \overline{t} be the vector with components t_0 , t_2 , t_3 , ..., $t_{2n+2h(n-1)}$ arranged in monotone non-decreasing order. Then wherever t_0 is, $M(\overline{g},\overline{t})$ is still non-singular. Since the solution to $M^T(\overline{g},\overline{t})$ $\overline{\alpha} = \overline{0}$ is $\overline{\alpha} = 0$, we see that only the trivial polynomial can have a 0 at all the components of \overline{t} . So P(x) has the property that it is 0 on

 $S(\mu)$, positive off $S(\mu)$ in the interval $[a,\beta_{n-1}]$, where β_{n-1} is the last mass point of μ in (ξ_h,b) , and negative on (β_{n-1},b) . Thus all points of $S(\mu')$ lie where $P(x) \geq 0$ and some lie where P(x) > 0. But if $\mu' \geq \mu$ it is necessary that $\int P(x) \ d(\mu' - \mu) = 0$. Since $\int P(x) \ d\mu' > 0$ and $\int P(x) \ d\mu = 0$, we have our contradiction and μ is admissible.

We now know that designs with more than (h+1)(n-1) points in (a,b) as well as non-permissible (h) designs are inadmissible. We know that designs that are permissible (h) and have (h+1)(n-1) or fewer points in (a,b) and miss the knots are admissible. If we could show that any permissible (h) design with (h+1)(n-1) or fewer points in (a,b) is admissible, we would have the following theorem- ''Let $n \geq 2$, k = n-2. Then a design μ is admissible if and only if μ is permissible (h) (or equivalently subadmissible (h)) and $S(\mu)$ has (h+1)(n-1) or fewer points in (a,b).'' Unfortunately, even though we suspect it is true, we cannot prove it. Instead we sum up the results of this section so far with

Theorem 15. Let $n \ge 2$, k = n-2.

- (1) Then if a design μ has (h+1)(n-1)+1 or more points of $S(\mu)$ in (a,b) it is inadmissible. Consistent with this, if μ is not permissible (h), μ is not subadmissible (h).
- (2) If μ is permissible (h) and has (h+l)(n-l) or fewer points of $S(\mu)$ in (a,b), none of them at a knot, then μ is admissible.

Notice that the class of admissible designs is contained in the class of permissible (h) designs with (h-1)(n-1) or fewer points in (a,b).

Example 4. Let n=2, k=0, h=2. Then we find all admissible designs by showing that any permissible (2) design μ with a,b and 3 points of (a,b) in $S(\mu)$ is admissible. If μ is such a design with no points

in (a,ξ_1) or (ξ_2,b) , Theorem 12 tells us μ is admissible. So we can restrict consideration to those μ with a point in both (a,ξ_1) and (ξ_2,b) . If the third point of $S(\mu)$ in (a,b) is in (ξ_1,ξ_2) , Theorem 15 tells us μ is admissible. So we need only consider the case when the third interior point of $S(\mu)$ is at one of the knots, say ξ_1 to be specific. Assume $\mu' \geq \mu$. Let α be the mass point of μ in (a,ξ_1) and β be the mass point of μ in (ξ_2,b) . By Lemma 9, there is a polynomial P(x) in $(x-\xi_1)^2_+,(x-\xi_1)^3_+,(x-\xi_2)^2_+,(x-\xi_2)^3_+$ that is 0 on $[a,\xi_1]$ and at the points of $S(\mu)$ in $[\xi_1b]$ and >0 off $S(\mu)$ in $[\xi_1,b]$ (see proof of Lemma 17). If $\mu' \geq \mu$, $S(\mu')$ would have to have a point in (ξ_2,b) to the left of β (see proof of Theorem 14). Thus P(x) d $\mu' > 0$ and P(x) d $\mu = 0$. This contradicts $\mu' \geq \mu$. The case where $\xi_2 \in S(\mu)$ is similar. Thus when n = 2, k = 0, n = 2 we can say ''A design μ is admissible if and only if it is permissible (2) and has fewer than 4 points in (a,b).''

Example 5. n=2, k=0, h=3. Here arguments similar to those in Example 4 give us that if μ is permissible (3) and has 4 points in (a,b), then μ is admissible-except in the case where the points of $S(\mu)$ lie in (a,ξ_1) and (ξ_3,b) and at ξ_1 and ξ_3 . In this latter case we don't know if μ is admissible or inadmissible.

5. Discussion and Conjecture

In this section we review some of the results we have, consider where generalizations breakdown, and offer a conjecture for the general solution to the problem.

First we reconsider the case where $n \ge 2$, k = n-2. It was mentioned that a permissible (h) design with (h+1)(n-1) points in (a,b) is admissible

if none of these points lie on knots. Notice that any permissible (h) design with (h+l)(n-l) points in (a,b) and some points at knots is the weak limit of a sequence of these admissible designs. It seems heuristically true that if one has a sequence of ''unbeatable'' designs, then the limit should be ''unbeatable.'' Unfortunately the analysis is not evident. In all the examples we have done no weak limits of admissible designs were known to be inadmissible. So we offer

Conjecture 1. Let $n \ge 2$ and k = n-2. Then a design is admissible if and only if it is permissible (h) and has fewer than (h+1)(n-1)+1 points in (a,b).

In the case where $n \ge 2$ and k = n-2 we were able to show, for each permissible (h) design μ with precisely $n + \frac{(n+k)h}{2}$ points in $S(\mu)$, all in (a,b), the existence of a set of polynomials $\{P_i(x)\}_{i=0}^h$ in $1,x,\ldots,$ $x^{2n-1},(x-\xi_1)_+^{n-k},\ldots,(x-\xi_1)_+^{2n-1},\ldots,(x-\xi_h)_+^{n-k},\ldots,(x-\xi_h)_+^{2n-1}$ and $f_i(x)$ where

$$f_o(x) = x^{2n} - (x - \xi_1)_+^{2n},$$

$$f_i(x) = (x - \xi_i)_+^{2n} - (x - \xi_{i+1})_+^{2n}, \quad i = 1, ..., h-1,$$

and

$$f_h(x) = (x-\xi_h)_+^{2n}$$

with the properties

(1) $P_i(x) = 0$ on $S(\mu)$ and $P_i(x) \neq 0$ on the points of $[\xi_i, \xi_{i+1}]$ not in $S(\mu)$,

- (2) the coefficient of $f_{i}(x)$ is 1,
- (3) $P_{i}(x) \ge 0$ or $P_{i}(x) \le 0$, and
- (4) $P_i(x) \ge 0$. (see Lemma 17)

In the case when n+k is even we are able to use Lemma 16 (as Lemma 8 was used to prove Lemma 14) and a generalization of Lemma 13 to get the existence of a set of polynomials for which we can presently verify all but property (4). If property (4) is true, analysis similar to that in Theorem 13 could be used to show

Conjectures 2. Let n+k be even. Then a design with n+h $\frac{(n+k)}{2}$ points in (a,b) is inadmissible.

If Conjecture 1 and 2 are true, I suspect that the next conjecture is also true.

Conjectures 3. Let n+k be even. Then a design is admissible if and only if it is permissible (h) and has fewer than n+h $(\frac{n+k}{2})$ points in (a,b). Notice that Conjecture 3 includes Conjectures 1 and 2.

We are now left with the problem of saying something about the case when n+k is odd, having little but Theorems 9 and 12 and Example 1 to drqw from. We notice in Theorem 12 that it is slightly ''easier'' for a design to be admissible when n+k is odd than when n+k is even, because the spectrum can have relatively more points in the end subintervals. Keeping this in mind, we make our final conjecture, which includes all the others.

Conjecture 4. A design is admissible if and only if it is subadmissible (h) and has fewer than $n+\frac{h(n+k)}{2}$ points in (a,b), unless it is subadmissible (h) and has $\frac{n+k-1}{2}$ or fewer points in either (a, ξ_1) or (ξ_h ,b). In this case it is admissible.

Note that for this latter case to apply n+k must be odd and $h \ge 2$. Recall Example 2, where n=3, k=0, h=2, and where a design with 6 points in (a,b) could be admissible. We suspect that some permissible (2) designs with 6 points in (a,b) are inadmissible, in particular those that have 0 mass at all the knots.

6. A Related Problem

In this section we discuss a generalization of the problem we've been considering. We have been trying to classify designs when the regression vector is $\overline{f}(x) = (1, x, \dots, x^n, (x - \xi_1)_+^{n-k}, \dots, (x - \xi_1)_+^n, \dots, (x - \xi_h)_+^{n-k}, \dots, (x - \xi_h)_+^n)^T$. Two of the basic results we've used readily generalize for the case where $\overline{f}(x) = (1, x, \dots, x^n, (x - \xi_1)_+^n, \dots, (x - \xi_1)_+^n, \dots, (x - \xi_h)_+^n)^T$, i.e., the case where the regression function is $n-k_1-1$ times differentiable at the knot ξ_1 . We state the results now.

Theorem 16. Let $\overline{f}(x)$ be as above. Let $\overline{g}(x) = (1,x,\ldots,x^{2n-1}, (x-\xi_1)_+^{n-k_1},\ldots,(x-\xi_h)_+^{2n-1},\ldots,(x-\xi_h)_+^{n-k_h},\ldots,(x-\xi_h)_+^{2n-1})^T$. Then $\mu' \geq \mu$ with respect to $\overline{f}(x)$ if and only if

(1)
$$\int \overline{g}(x) d(\mu^{\tau} - \mu) = 0$$
 and

(2)
$$0 \neq \int x^{2n} d(\mu' - \mu) \geq \int (x - \xi_1)_+^{2n} d(\mu' - \mu) \geq \dots \geq \int (x - \xi_h)_+^{2n} d(\mu' - \mu) \geq 0.$$

where no more than $(s-\ell_1+1)$ t values are ξ_1 , where no more than (s+1) t values coincide. Then $M(\overline{f},\overline{t})$ is non-singular if and only if

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