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Recurrence Moment Formulas for *D*-optimal Designs

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ABSTRACT. We derive recurrence formulas for the moments of the *D*-optimal designs for the polynomial model of degree *k* under different assumptions on the heteroscedastic structure. A new proof for deriving the asymptotic optimal designs as *k* tends to infinity is given. We also show these recurrence formulas are useful for identifying the asymptotic optimal designs in other settings, including limiting model robust optimal designs.

Key words: approximate designs, asymptotic distributions, model robust optimal designs, efficiency functions, orthogonal polynomials

1. Introduction

This research is largely motivated by several recent results in the statistical literature that are derived from moment recurrence formulas. Hoffmann & Schmidt (1982) characterized the exponential family using recurrence relations of moments. Likewise Cobb *et al.* (1983) used moment recurrence relations for estimating parameters in the exponential family with multimodal distributions. Recurrence formulas are particularly useful in distribution theory; see for example Gleissner (1984), Bowman & Shenton (1986), Lindsay (1989 *a*, *b*) and Schröter (1990). More recently, Drane *et al.* (1993) established via recurrence formulas that many common discrete distributions are limiting forms of the Polya–Eggenberger distribution. Applications to practical problems relying on recurrence formulas can be found in Bassukas and Mauerer-Schultze (1988).

The goal of this paper is to provide an alternative approach to studying properties of *D*-optimal designs in weighted polynomial regression. We derive moment recurrence formulas for these designs and give a new proof for the asymptotic *D*-optimal designs for the polynomial model of degree k as k tends to infinity for various efficiency functions. While the asymptotic results are not new (Kiefer & Studden, 1976; Studden, 1980, 1982 *b*; Lau, 1988), the methodology is illuminating and potentially useful for study of optimal designs, particularly their limiting properties. Two such applications are briefly indicated in the last section.

2. Background

We assume a linear model with a known regression function given by $f_k^T(x) = (1, x, x^2, \ldots, x^k)$ defined on some given interval Ω. It is further assumed that for each $x \in \Omega$, the univariate response $y(x)$ is observed with an error $e(x)$ having mean zero and variance proportional to $1/\lambda(x)$. The statistical model is

$$y(x) = f_k^T(x)\beta + e(x) \quad x \in \Omega.$$

Here β is the vector of parameters and the non-negative function $\lambda(x)$ is usually called the efficiency function. Thus, we have a heteroscedastic model whenever $\lambda(x)$ is not constant

across Ω. All designs considered here are approximate in the sense that they are viewed as probability measures defined on Ω. Following standard convention, we measure the information contained in a design ξ by its information matrix,

$$M_k(\xi) = \int_\Omega f_k(x) f_k^T(x) \lambda(x) \xi(dx),$$

which for our purposes here, will be assumed to be non-singular. For expository purposes, we shall concentrate on the following efficiency functions.

(a) $\lambda_1(x) = 1$ $\Omega = [-1, 1]$;

(b) $\lambda_2(x) = (1-x)^{\alpha+1}(1+x)^{\beta+1}$ $\Omega = [-1, 1]$, $\alpha > -1$, $\beta > -1$;

(c) $\lambda_3(x) = \exp(-x)$ $\Omega = [0, \infty)$;

(d) $\lambda_4(x) = x^{\alpha+1} \exp(-x)$ $\Omega = [0, \infty)$, $\alpha > -1$;

(e) $\lambda_5(x) = \exp(-x^2)$ $\Omega = (-\infty, \infty)$.

If the main interest in the experiment is to estimate the parameters in the model, a reasonable criterion is D-optimality. This criterion seeks a design which maximizes the determinant of the information matrix over the set of all designs defined on Ω. Such designs are called D-optimal designs and they are popular in practice. The D-optimal designs for the above efficiency functions are given in Karlin & Studden (1966), Fedorov (1972, p. 88) and Studden (1982 *b*). For convenience, the D-optimal design for the model $f_k(x)$ with efficiency function $\lambda_i(x)$ is denoted by $\xi_{k,i}$, $i = 1, 2, 3, 4, 5$. Discussion on the motivation and other properties of the D-optimality criterion can be found in Kiefer (1985) and the references therein.

3. Recurrence moment formulas for D-optimal designs

There is a vast amount of work on approximate D-optimal designs, see Kiefer (1985). In particular, it is known that for all k and $i = 1, 2, 3, 4, 5$, $\xi_{k,i}$ is equally supported at $k+1$ points given by zeros of certain polynomials. However, the following moment recurrence formulas of these designs appear to be unknown.

Theorem 3.1

Let $\mu_{r,k}$ be the rth moment of the D-optimal design for one of the efficiency functions listed in section 2. The following recurrence formulas hold:

(*a*) $\lambda_1(x) = 1$

(i) $\mu_{2r-1,k} = 0$;

(ii) $$\mu_{2r,k} = \frac{1}{2k+1-2r}\left\{k - (k+1)\sum_{v=1}^{r-1} \mu_{2r-2v,k}\mu_{2v,k}\right\} \quad r = 1, 2, 3, \ldots$$

(*b*) $\lambda_2(x) = (1-x)^{\alpha+1}(1+x)^{\beta+1}$, $\alpha > -1, \beta > -1$.

(i) $$\mu_{1,k} = \frac{\beta - \alpha}{2k+\alpha+\beta+2};$$

(ii) $$\mu_{r,k} = \frac{1}{2k+\alpha+\beta+3-r}\left\{(k+1)\sum_{v=0}^{r-2} \mu_{r-2-v,k}\mu_{v,k} - (k+1)\sum_{v=1}^{r-1} \mu_{r-v,k}\mu_{v,k} + (\beta-\alpha)\mu_{r-1,k} - (r-1)\mu_{r-2,k}\right\} \quad r = 2, 3, 4, \ldots$$

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(*c*) $\lambda_3(x) = \exp(-x)$

(i) $\mu_{1,k} = \dfrac{k^2}{k+1}$;

(ii) $\mu_{r,k} = (k+1)\sum_{v=1}^{r-2} \mu_{r-1-v,k}\mu_{v,k} + (1-r+2k)\mu_{r-1,k} \quad r = 2, 3, 4, \ldots$

(*d*) $\lambda_4(x) = x^{\alpha+1}\exp(-x)$, $\alpha > -1$.

$$\mu_{r,k} = (k+1)\sum_{v=0}^{r-1} \mu_{r-1-v,k}\mu_{v,k} + (\alpha+1-r)\mu_{r-1,k} \quad r = 1, 2, 3, \ldots$$

(*e*) $\lambda_5(x) = \exp(-x^2)$

(i) $\mu_{2r-1,k} = 0$;

(ii) $\mu_{2r,k} = \dfrac{1}{2}\left\{(k+1)\sum_{v=0}^{r-1} \mu_{2r-2v-2,k}\mu_{2v,k} - (2r-1)\mu_{2r-2,k}\right\} \quad r = 1, 2, 3, \ldots$

Proof. We provide only the proof for case (a) since the others follow similarly. Let $L_k(x)$ be the kth order Legendre polynomial, $L_k'(x)$ be its derivative and $s_1, s_2, \ldots, s_{k+1}$ be the zeros of $g_k(x) = (1-x^2)L_k'(x)$, which are all located in the interval $[-1, 1]$. Since the D-optimal design puts equal mass at $s_1, s_2, \ldots, s_{k+1}$,

$$\mu_{r,k} = \frac{1}{k+1}\sum_{i=1}^{k+1} s_i^r.$$

From Abramowitz & Stegun (1966, p. 781; (22.6.3)), we have $(1-x^2)g_k''(x) = -k(k+1)g_k(x)$ and it follows that if $x \neq 0$ and $x \neq s_i$ for $i = 1, 2, \ldots, k+1$,

$$-\frac{k(k+1)}{1-x^2} = \frac{g_k''(x)}{g_k(x)} = \sum_{1 \leq i \neq j \leq k+1} \frac{1}{(x-s_i)(x-s_j)}$$

or

$$\frac{k(k+1)}{x^2\left(1-\dfrac{1}{x^2}\right)} = \sum_{1 \leq i \neq j \leq k+1} \left(\frac{1}{1-\dfrac{s_i}{x}} - \frac{1}{1-\dfrac{s_j}{x}}\right)\frac{1}{x(s_i-s_j)}.$$

Expanding both sides as power series in $x^{-2}(|x| > 1)$ yields

$$k(k+1)\sum_{v=0}^{\infty} \frac{1}{x^{2v+2}} = \sum_{1 \leq i \neq j \leq k+1} \sum_{v=0}^{\infty} \frac{s_i^v - s_j^v}{x^{v+1}(s_i-s_j)} = \sum_{v=0}^{\infty} \frac{1}{x^{1+v}} \sum_{1 \leq i \neq j \leq k+1} \frac{s_i^v - s_j^v}{s_i - s_j}.$$

Clearly from the above equation, all odd moments of the design are zero, proving part (i) of case (a). Part (ii) follows by noting that for even powers of x,

$$\begin{aligned} k(k+1) &= \sum_{1 \leq i \neq j \leq k+1} \sum_{v=0}^{2r} s_i^{2r-v}s_j^v = \sum_{j=1}^{k+1}\sum_{i=1}^{k+1}\sum_{v=0}^{2r} s_i^{2r-v}s_j^v - \sum_{i=1}^{k+1}\sum_{v=0}^{2r} s_i^{2r} \\ &= (k+1)\left\{(k+1)\sum_{v=0}^{2r} \mu_{2r-v,k}\mu_{v,k} - (2r+1)\mu_{2r,k}\right\} \\ &= (k+1)\left\{(k+1)\sum_{v=0}^{r-1} \mu_{2r-2v,k}\mu_{2v,k} + (2k-2r+1)\mu_{2r,k}\right\}, \end{aligned}$$

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thus completing the proof of the theorem. Cases (b)–(e) are proved analogously with the formulas (22.6.1), (22.6.15) and (22.6.19) from Abramowitz & Stegun (1966). □

The results in theorem 3.1 are quite remarkable in that the rth moments of the D-optimal designs for $f_k(x)$ can be written explicitly in terms of r and k without explicit knowledge of the support points of the designs. For instance, if the efficiency function is $\lambda_1(x)$ and k is a positive integer, we have

$$\mu_{2,k} = \frac{k}{2k-1}, \quad \mu_{4,k} = \frac{k(3k^2-5k+1)}{(2k-3)(2k-1)^2},$$

and

$$\mu_{6,k} = \frac{k(10k^4-44k^3+56k^2-22k+3)}{(2k-5)(2k-3)(2k-1)^3}.$$

It is notable that the proof of theorem 3.1 does not rely on the theory of canonical moments, which is a common tool for studying D-optimal designs in polynomial regression, see Studden (1980, 1982 *a*, *b*). Consequently, theorem 3.1 may be used to provide alternative proofs of results for D-optimal designs. We illustrate this here by establishing the asymptotic D-optimal designs of $\xi_{k,i}$ as k tends to infinity for $i = 1, 2, 3, 4, 5$. A different proof of this result is given in Gawronski (1987) and Lau (1988).

Theorem 3.2

Let $F_k(x)$ denote the distribution function of the D-optimal design for the polynomial model of degree k with one of the efficiency functions listed in section 2.

(i) *If* $\lambda_1(x) = 1$ *or* $\lambda_2(x) = (1-x)^{\alpha+1}(1+x)^{\beta+1}$,

$$\lim_{k\to\infty} F_k(x) = \frac{1}{\pi}\int_{-1}^{x} \frac{1}{\sqrt{1-t^2}}\,dt, \quad x \in [-1, 1];$$

(ii) $\lambda_3(x) = \exp(-x)$ *or* $\lambda_4(x) = x^{\alpha+1}\exp(-x)$

$$\lim_{k\to\infty} F_k(4kx) = \frac{2}{\pi}\int_{0}^{x} \sqrt{\frac{1-t}{t}}\,dt, \quad x \in [0, 1];$$

(iii) $\lambda_5(x) = \exp(-x^2)$

$$\lim_{k\to\infty} F_k(\sqrt{2k}\,x) = \frac{2}{\pi}\int_{-1}^{x} \sqrt{1-t^2}\,dt, \quad x \in [-1, 1].$$

Proof. Since the proofs are quite similar to all the cases, we provide details for the cases when the efficiency function is $\lambda_2(x)$ and $\lambda_5(x)$. The key idea is to show the limiting design can be uniquely identified by the limit of the moment sequence of the D-optimal designs for model $f_k(x)$. This is accomplished by induction on the rth moment of the optimal design via the recurrence formulas from theorem 3.1. and letting k go to infinity. The rest of the argument, including the uniqueness of the asymptotic design follows from Wilks (1962, p. 126).

Case (i). $\lambda_2(x) = (1-x)^{\alpha+1}(1+x)^{\beta+1}$.

We claim that the limiting moments are the moments of the arc-sine distribution given by $\{\gamma_r\}_{r\geq 1}$ where

$$\lim_{k\to\infty} \mu_{j,k} = \gamma_j = \begin{cases} 0 & \text{if } j \text{ is odd} \\ \dfrac{\Gamma(r+\frac{1}{2})}{\Gamma(r+1)\Gamma(\frac{1}{2})} & \text{if } j = 2r \text{ is even.} \end{cases}$$

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From theorem 3.1(b),

$$\lim_{k\to\infty}\mu_{1,k}=\lim_{k\to\infty}\frac{\beta-\alpha}{2k+\alpha+\beta+2}=0=\gamma_1$$

$$\lim_{k\to\infty}\mu_{2,k}=\lim_{k\to\infty}\frac{1}{2k+\alpha+\beta+1}\left\{(k+1)-(k+1)\frac{(\beta+\alpha)^2}{(2k+\alpha+\beta+2)^2}\right.$$

$$\left.+\frac{(\beta-\alpha)^2}{2k+\alpha+\beta+2}-1\right\}=\tfrac{1}{2}=\gamma_2.$$

If the moments are odd, from theorem 3.1(b) and induction,

$$\lim_{k\to\infty}\mu_{2r+1,k}=\frac{1}{2}\left\{\sum_{v=0}^{2r-1}\gamma_{2r-1-v}\gamma_v-\sum_{v=1}^{2r}\gamma_{2r+1-v}\gamma_v\right\}=0$$

since every summand in each of these sums contains an odd index. If the moments are even,

$$\lim_{k\to\infty}\mu_{2r,k}=\frac{1}{2}\left\{\sum_{v=0}^{2r-2}\gamma_{2r-2-v}\gamma_v-\sum_{v=1}^{2r-1}\gamma_{2r-v}\gamma_v\right\}=\frac{1}{2}\left\{\sum_{v=0}^{r-1}\gamma_{2r-2-2v}\gamma_{2v}-\sum_{v=1}^{r-1}\gamma_{2r-2v}\gamma_{2v}\right\}$$

$$=\tfrac{1}{2}\Gamma\left(\frac{1}{2}\right)^{-2}\left\{\sum_{v=0}^{r-1}\frac{\Gamma(r-v-\frac{1}{2})}{\Gamma(r-v)}\frac{\Gamma(v+\frac{1}{2})}{\Gamma(1+v)}-\sum_{v=0}^{r}\frac{\Gamma(r-v+\frac{1}{2})}{\Gamma(r-v+1)}\frac{\Gamma(v+\frac{1}{2})}{\Gamma(1+v)}\right.$$

$$\left.+2\frac{\Gamma(\frac{1}{2})\Gamma(r+\frac{1}{2})}{\Gamma(r+1)}\right\}$$

$$=\tfrac{1}{2}\Gamma\left(\frac{1}{2}\right)^{-2}\left\{\Gamma\left(\frac{1}{2}\right)^2-\Gamma\left(\frac{1}{2}\right)^2+2\frac{\Gamma(\frac{1}{2})\Gamma(r+\frac{1}{2})}{\Gamma(r+1)}\right\}=\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})\Gamma(r+1)}.$$

Here, the second to the last equality holds because of lem. 4.1 in Dette (1990). The proof for $\lambda_2(x)=(1-x)^{\alpha+1}(1+x)^{\beta+1}$ is complete.

Case (ii): $\lambda_5(x)=\exp(-x^2)$.

It is known that the D-optimal design for the polynomial regression model of degree k puts equal mass at the zeros of the Hermite polynomial $H_{k+1}(x)$ of degree $k+1$. These polynomials are orthogonal with respect to the measure $\exp(-x^2)\,dx$ over the region $(-\infty,\infty)$. Accordingly, let U_k be the uniform distribution on $\{(x/\sqrt{2k})\mid H_{k+1}(x)=0\}$ and define $m_{r,k}=\int x^r\,dU_k(x)$, $r\geqslant 1$. Clearly $m_{j,k}=0$ if i is odd and $m_{2r,k}=\mu_{2r,k}/(2k)^r$ where $\mu_{r,k}$ is the rth moment of $\xi_{k,5}$. We claim that the limiting moments are given by γ_{2r}, where

$$\lim_{k\to\infty}m_{2r,k}=\frac{2}{\pi}\int_{-1}^{1}x^{2r}\sqrt{1-x^2}\,dx=\binom{2r}{r}\frac{1}{r+1}\frac{1}{2^{2r}}=\gamma_{2r}$$

Proof. If $r=1$ or 2,

$$\lim_{k\to\infty}m_{2,k}=\lim_{k\to\infty}\frac{1}{2k}\mu_{2,k}=\frac{1}{4}=\gamma_2$$

and

$$\lim_{k\to\infty}m_{4,k}=\lim_{k\to\infty}\frac{1}{4k^2}\mu_{4,k}=\lim_{k\to\infty}\frac{2k-1}{4k^2}\frac{k}{4}=\frac{1}{8}=\gamma_4.$$

Furthermore, theorem 3.1(e) implies

$$m_{2r+2,k}=\frac{1}{2}\left\{\frac{k+1}{2k}\sum_{v=0}^{r}m_{2r-2v,k}m_{2v,k}-\frac{2r+1}{2k}m_{2r,k}\right\}$$

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and by induction,

$$\lim_{k\to\infty} m_{2r+2,k} = \frac{1}{2}\left\{\frac{1}{2}\sum_{v=0}^{r}\gamma_{2r-2v}\gamma_{2v}\right\} = \frac{1}{4}\sum_{v=0}^{r}\frac{1}{2^{2r}}\binom{2v}{v}\binom{2r-2v}{r-v}\frac{1}{v+1}\frac{1}{r-v+1}$$

$$= \frac{1}{2^{2r+2}}\binom{2r+2}{r+1}\frac{1}{r+2} = \gamma_{2r+2}.$$

The second to last equality follows from the expansion

$$\sum_{v=0}^{\infty}\binom{2v}{v}\frac{x^v}{v+1} = \frac{1-\sqrt{1-4x}}{2x} \tag{3.1}$$

and comparing the coefficient of x^r in the following equation obtained by squaring both sides of (3.1):

$$\sum_{r=0}^{\infty}\left\{\sum_{v=0}^{r}\binom{2v}{v}\binom{2r-2v}{r-v}\frac{1}{v+1}\frac{1}{r-v+1}\right\}x^r = \frac{1-\sqrt{1-4x}}{2x^2} - \frac{1}{x}$$

$$= \frac{1}{x}\sum_{r=0}^{\infty}\binom{2r}{r}\frac{x^r}{r+1} - \frac{1}{x}$$

$$= \sum_{r=0}^{\infty}\left\{\binom{2r+2}{r+1}\frac{1}{r+2}\right\}x^r.$$

This completes the proof of theorem 3.2. □

Using similar techniques, limiting distributions of D-optimal designs for other classes of efficiency functions described in Lau and Studden (1988) can be found and shown to have similar limit distributions as in theorem 3.2. The next section shows the model robust designs in Dette (1990) also satisfy similar recursive relations and have the arc-sine distribution as the limiting distribution.

4. Applications

In this section, we briefly discuss how our results may be applied to obtain asymptotic or limiting optimal designs in two other settings. Following Läuter (1974), we define a design ξ^* on the interval $[-1, 1]$ to be optimal for the class of polynomials up to degree k if ξ^* maximizes the criterion

$$\Phi_\beta(\xi) = \sum_{i=1}^{k}\beta_i \log|M_i(\xi)|. \tag{4.1}$$

Here $\beta^T = (\beta_1, \beta_2, \ldots, \beta_k)$ denotes a prior which reflects the experimenter's belief about the adequacy of the different models. If $z \geqslant 0$, consider the prior $\beta(z) = (\beta_1(z), \beta_2(z), \ldots, \beta_k(z))$ with

$$\beta_i(z) = \Gamma(k+z-i-1)\sigma/\Gamma(k+1-i), \quad i = 1, 2, \ldots, k,$$

and σ is such that $\Sigma_{i=1}^{k}\beta_i(z) = 1$. Dette (1990) showed that the design ξ_z^* maximizing (4.1) has equal mass $1/(k+z)$ at the $k-1$ zeros of the Jacobi polynomial $P_{k-1}^{((z+1)/2,\,(z+1)/2)}(x)$ and mass $(z+1)/(2k+2z)$ at each of the endpoints -1 and 1. When k is large, it may be of interest to investigate the asymptotic behavior of this design. To this end, assume $z = z_k = ak + o(k)$ and $a \geqslant 0$.

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The moments $\eta_{r,k}$ of $\xi^*_{z_k}$ for $k > 2$ are given by

$$\eta_{r,k} = \frac{k-1}{k+z_k}\mu_{r,k-2} + \frac{z_k+1}{2(k+z_k)}\{1+(-1)^r\},$$

where $\mu_{r,k-2}$ is the rth moment of the uniform distribution on the zeros of the Jacobi polynomial $P_{k-1}^{((z+1)/2,(z+1)/2)}(x)$. Using theorem 3.1(b), a straightforward analysis shows all the odd moments of $\xi^*_{z_k}$ vanish and the even moments satisfy the recursive relation

$$\eta_{2r,k} = \frac{1}{2k+z_k-2r}\left\{(k+z_k)\sum_{i=0}^{r-1}\eta_{2r-2-2i,k}\eta_{2i,k} - (k+z_k)\sum_{i=1}^{r-1}\eta_{2i,k}\eta_{2r-2i,k} - (2r-1)\eta_{2r-2,k}\right\}.$$

If $r \geqslant 1$, and $k \to \infty$ such that $z_k/k \to a \geqslant 0$, we have

$$\mu^*_{2r} = \frac{a+1}{a+2}\left\{\sum_{i=0}^{r-1}\mu^*_{2r-2-2i}\mu^*_{2i} - \sum_{i=1}^{r-1}\mu^*_{2r-2i}\mu^*_{2i}\right\}.$$

Using similar but slightly more complicated arguments as in the proof of theorem 3.2, the measure ξ^* corresponding to this sequence of moments can be shown to be unique with an absolute continuous component (with respect to the Lebesgue measure) given by

$$\frac{d\xi^*}{dx} = \frac{1}{\pi}\frac{\sqrt{(a+1)-(1+a/2)^2x^2}}{(a+1)(1-x^2)} I\left\{|x| \leqslant \frac{\sqrt{a+1}}{1+a/2}\right\}$$

and two additional jumps of order $a/(2a+2)$ at the points -1 and 1.

Note that if $a = 0$, we have the arc-sine limit distribution while for larger values of a, the limit distribution is more concentrated at the extreme points -1 and 1. This corresponds to the intuition that for large values of z, the prior $\beta(z)$ puts more weight on the polynomials of lower degrees.

Another application of the results in section 3 is to consider the setup in theorem 3.2 but this time we permit the parameters in the efficiency function to vary. For example, if $\lambda(x) = x^{ak}\exp(-x)$ $(x > 0, a \geqslant 0)$, an application of theorem 3.1(d) shows the distribution function $F_k(x)$ of the D-optimal design for $f_k(x)$ with this efficiency function satisfies

$$\lim_{k\to\infty} F_k(kx) = \frac{1}{2\pi}\int_{r_1}^{x}\frac{\sqrt{(r_2-t)(t-r_1)}}{t}\,dt \quad r_1 \leqslant x \leqslant r_2$$

where $r_i = 2 + a + (-1)^i\sqrt{1+a}$, $i = 1, 2$. Analogous results for the other efficiency functions of theorem 3.1 are omitted for the sake of brevity.

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