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EXACT ELFVING-MINIMAX DESIGNS FOR QUADRATIC REGRESSION

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Abstract. For quadratic polynomial regression on [-1, 1] exact *n*-point designs are given which minimize the maximal variance of the estimated parameters. It turns out that they coincide with *c*-optimum designs for estimating the parameter with highest degree.

Key words and phrases: Exact regression designs, Elfving-optimality, *c*-optimal designs.

1. Introduction and Notations

In this paper we present exact optimum designs for a minimax criterion first proposed by Elfving (1959), here restricted to the case of quadratic polynomial regression on the interval [-1, 1]. This means explicitly: Let

$$y(x) = a_1 + a_2 x + a_3 x^2, \quad x \in [a, b].$$

Assume that for each component x_i of $\mathbf{x} = (x_1, x_2, \dots, x_n) \in [a, b]^n$ one can observe random variables Y_{x_i} which have expectations $E(Y_{x_i}) = y(x_i)$, variances $\operatorname{Var}(Y_{x_i}) = \sigma^2$, independent of x_i , and which are pairwise uncorrelated. Such a vector \mathbf{x} is called an exact *n*-point design d_n .

We use the notations

$$s_{\nu} = s_{\nu}(d_n) = \sum_{j=1}^n x_j^{\nu}, \quad 0 \le \nu \le 4,$$
$$M(d_n) = \begin{bmatrix} s_0 & s_1 & s_2\\ s_1 & s_2 & s_3\\ s_2 & s_3 & s_4 \end{bmatrix}$$

and

$$\Delta_n = \{ d_n : M(d_n) \text{ is regular} \}.$$

Note that det $M(d_n)$ is the sum of squares of Vandermonde determinants. Hence $d_n \in \Delta_n$ if and only if d_n has at least three different components.

It is well-known that for $d_n \in \Delta_n$ the covariance matrix of the least squares estimator $\hat{\mathbf{a}} = (\hat{a}_1, \hat{a}_2, \hat{a}_3)^T$ of $\mathbf{a} = (a_1, a_2, a_3)^T$ is given by

$$Cov(\hat{\mathbf{a}}) = \sigma^2 M^{-1}(d_n) = \sigma^2 (m^{ij}(d_n))_{1 \le i, j \le 3},$$

in particular, $\operatorname{Var}(\hat{a}_i) = \sigma^2 m^{ii}(d_n), \ 1 \le i \le 3.$

We call a design $d_n^* \in \Delta_n$ an *n*-point EMM-design (Elfving-minimax design, cf. Elfving (1959)) iff it satisfies

$$\max_{1 \le i \le 3} m^{ii}(d_n^*) \le \max_{1 \le i \le 3} m^{ii}(d_n) \quad \text{for all} \quad d_n \in \Delta_n.$$
(1)

In Section 2 we present the *n*-point EMM-designs for the case [a, b] = [-1, 1].

It will turn out that in this special setting EMM-optimality is equivalent to c-optimality for $c = e_3 = (0, 0, 1)^T$. In the approximate theory the c-optimal design is well-known in more general settings. Unfortunately, the methods applied there are not appropriate in the exact theory. For instance, the minimax theorem in the remarkable paper (Kiefer and Wolfwitz (1959)) does not hold in the exact theory. Our results also provide an example for the difference between approximate and exact optimal designs; here, even the support of the optimal exact design may differ from that of the optimal approximate design. Apparently, a first example of this type is the exact G-optimal design for linear regression when n is odd, cf. Jung (1971).

2. *n*-Point EMM-Designs

We consider the setting given in the introduction with [a, b] = [-1, 1]. The symmetry of the problem suggests that the optimum design should be symmetric around zero. Putting n = 4p+q, $q \in \{0, 1, 2, 3\}$, it came as a surprise to us that for q = 2 this is not the case. In fact, this case requires a rather involved analysis. We therefore give the solution for the other cases first. (A design $d_n = (x_1, x_2, \ldots, x_n)$ for which n_i components are equal to a_i , $1 \le i \le 3$, $n_1 + n_2 + n_3 = n$, will be denoted by

$$d_n = \begin{bmatrix} a_1 & a_2 & a_3 \\ n_1 & n_2 & n_3 \end{bmatrix})$$

Proposition 1. Let n = 4p + q, $p \in \mathbb{N}$, $q \in \{0, 1, 3\}$ (or p = 0 and q = 3). Then the n-point EMM-designs are uniquely determined and given by

$$\begin{aligned} d_n^* &= \begin{bmatrix} -1 & 0 & 1 \\ p & 2p & p \end{bmatrix}, & n = 4p, \\ d_n^* &= \begin{bmatrix} -1 & 0 & 1 \\ p & 2p + 1 & p \end{bmatrix}, & n = 4p + 1, \\ d_n^* &= \begin{bmatrix} -1 & 0 & 1 \\ p + 1 & 2p + 1 & p + 1 \end{bmatrix}, & n = 4p + 3. \end{aligned}$$

Proof. Let $d_n \in \Delta_n$. Then we have

$$m^{33}(d_n) = (ns_2 - s_1^2) \det M^{-1}(d_n) \ge n(ns_4 - s_2^2)^{-1}.$$
 (2)

This follows at once from $(ns_2 - s_1^2)(ns_4 - s_2^2) - n \det M(d_n) = (ns_3 - s_1s_2)^2$. For d_n^* one easily obtains

$$\max_{1 \le i \le 3} m^{ii}(d_n^*) = \begin{cases} p^{-1}, & \text{if } n = 4p, \\ n(2p(2p+1))^{-1}, & \text{if } n = 4p+1, \\ n((2p+1)(2p+2))^{-1}, & \text{if } n = 4p+3. \end{cases}$$
(3)

Putting $y_i = x_i^2$, one observes that $v(y_1, y_2, ..., y_n) = n \sum_{i=1}^n y_i^2 - \left[\sum_{i=1}^n y_i\right]^2 = ns_4 - s_2^2$ is convex on $[0, 1]^n$. Thus, v attains its maximum only for $y_i^* \in \{0, 1\}$, $1 \le i \le n$. Let $r = r(y_1^*, y_2^*, ..., y_n^*) = \#\{i : y_i^* = 1\}$. Then

$$\begin{cases} 4p^2 - v(y_1^*, y_2^*, \dots, y_n^*) = (2p - r)^2 \ge 0, & \text{if } n = 4p, \\ 2p(2p + 1) - v(y_1^*, y_2^*, \dots, y_n^*) = (r - 2p)(r - 2p - 1) \ge 0, & \text{if } n = 4p + 1, \\ (2p + 1)(2p + 2) - v(y_1^*, y_2^*, \dots, y_n^*) = (r - 2p - 1)(r - 2p - 2) \ge 0, & \text{if } n = 4p + 3. \end{cases}$$
(4)

Combining (2), (4) and (3), yields

$$\max_{1 \le i \le 3} m^{ii}(d_n) \ge m^{33}(d_n) \ge \max_{1 \le i \le 3} m^{ii}(d_n^*).$$

One also gets uniqueness of d_n^* by discussing the cases when equality holds in (2) and (4).

In the same way as for the case n = 4p one can show that the approximate EMM-design is given by $\zeta^*(-1) = \zeta^*(1) = 1/4$, $\zeta^*(0) = 1/2$. It is thus the same as the approximate A-optimum design.

For the case n = 4p + 2 the technique used in the proof of Proposition 1 does not go through. Our approach will proceed by deriving some "completeclass-type" results whose proof is - in view of their quite technical structure - postponed to the appendix. We first show that one can restrict oneself to designs of the form

$$d_n = \begin{bmatrix} -1 & x & 1\\ k & m & \ell \end{bmatrix}, \quad x \in (-1, 1), \quad k, \, \ell, m \in \mathbb{N}.$$
(5)

We then prove that in case n = 4p + 2 a design of the form (5) cannot be an EMM-design if $k + \ell \neq 2p + 1$. Finally, we treat the case $k + \ell = 2p + 1$ and get

Proposition 2. Let n = 4p + 2 and x_0 be the real root of u(x) = 0, where

$$u(x) = (2p+1)^2 x^3 - 3(2p+1)x^2 + (20p^2 + 20p + 3)x - 2p - 1.$$
 (6)

Then

$$d_n^* = \begin{bmatrix} -1 & x_0 & 1 \\ p & 2p+1 & p+1 \end{bmatrix} and d_n^{**} = \begin{bmatrix} -1 & -x_0 & 1 \\ p+1 & 2p+1 & p \end{bmatrix}$$

are the n-point EMM-designs.

Remark. A referee asked for a generalization to arbitrary intervals [a, b]. This seems to be formidable as one can already guess from the structure of the approximate EMM-design for linear regression: It has support $\{a, b\}$ and weights

$$\begin{split} \zeta(a) &= \zeta(b) = \frac{1}{2}, & \text{if } a^2 + b^2 \leq 2, \\ \zeta(a) &= |b|(|a| + |b|)^{-1}, \, \zeta(b) = 1 - \zeta(a), & \text{if } |ab| \geq 1, \\ \zeta(a) &= (1 - b^2)(a^2 - b^2)^{-1}, \, \zeta(b) = 1 - \zeta(a), & \text{otherwise.} \end{split}$$

If one considers, however, only $c = (0, 0, 1)^T$ -optimal designs, then from propositions 1 and 2 one gets also the solution for arbitrary intervals [a, b], simply by transformation of the support. In the case of symmetric intervals [-b, b] an inspection of the proofs reveals that slight extensions are possible. So Proposition 1 remains true, if one replaces the support by $\{-b, 0, b\}$ and b is such that

$$\begin{split} b^4 &\leq 2, & \text{if } n = 4p, \\ b^4 &\leq (2p)^{-1}(4p+1), & \text{if } n = 4p+1, \\ b^4 &\leq (2(p+1))^{-1}(4p+3), & \text{if } n = 4p+3. \end{split}$$

In case n = 4p + 2, b^4 also has to be upper bounded by a function f(p) which is too involved to be reproduced here.

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Appendix

Several lemmas will be necessary to prove Proposition 2. The first lemma shows that for d_n^* , d_n^{**} one has

$$\max_{1 \le i \le 3} m^{ii}(d_n^*) = m^{33}(d_n^*) = m^{33}(d_n^{**}) = \max_{1 \le i \le 3} m^{ii}(d_n^{**}).$$
(7)

As a consequence we only have to show that

$$m^{33}(d_n^*) \le m^{33}(d_n)$$
 for all $d_n \in \Delta_n$. (8)

Lemma 1.

(a) The polynomial u(x) from (6) has exactly one real root x_0 and $x_0 \in (0, 1)$.

(b) For d_n^* , d_n^{**} as given in Proposition 2 the relations (7) hold true.

Proof. (a) One easily checks that the derivative u'(x) is positive for all $x \in \mathbb{R}$ and that u(0) < 0 < u(1). This implies (a).

(b) For $x_i \in [-1, 1]$, $1 \le i \le n$, one always has

$$2(ns_2 - s_1^2 - s_2s_4 + s_3^2) = \sum_{i=1}^n \sum_{j=1}^n (x_i - x_j)^2 (1 - x_i^2 x_j^2) \ge 0,$$

hence

$$m^{33}(d_n) > m^{11}(d_n)$$
 for all $d_n \in \Delta_n$.

Furthermore, d_n^* satisfies

$$(4p+2)s_2(d_n^*) - (s_1(d_n^*))^2 - (4p+2)s_4(d_n^*) + (s_2(d_n^*))^2 = (2p+1)^2 x_0^2 (1-x_0^2) + ((2p+1)x_0 - 1)^2 + (2p+1)^2 x_0^2 + 4p(p+1) - 1 > 0,$$

hence

$$m^{33}(d_n^*) > m^{22}(d_n^*).$$

The arguments for d_n^{**} are the same.

It remains to prove (8). Here the crucial step is to show that for a design $\hat{d}_n = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_n)$ minimizing $m^{33}(d_n)$ necessarily all $\hat{x}_i \in (-1, 1)$ have to be the same. This will be proved by considering the derivatives w.r.t. \hat{x}_i all other \hat{x}_j kept fixed. The following notations are useful:

Let $n \in \mathbb{N}, n \ge 3, x_1, x_2, \dots, x_n \in \mathbb{R}$ be given, $d_n = (x_1, x_2, \dots, x_n)$ and for $x \in \mathbb{R}$

$$d_x = (x_1, x_2, \dots, x_n, x),$$
$$M(d_x) = M + F(x),$$

where

$$M = M(d_n) = \begin{bmatrix} n & s_1 & s_2 \\ s_1 & s_2 & s_3 \\ s_2 & s_3 & s_4 \end{bmatrix}, \quad F(x) = \begin{bmatrix} 1 & x & x^2 \\ x & x^2 & x^3 \\ x^2 & x^3 & x^4 \end{bmatrix}.$$

Furthermore, let

$$D = \{x \in \mathbb{R} : M(d_x) \text{ is regular}\}\$$

and

$$\varphi(x) = m^{33}(d_x) = e_3^T M^{-1}(d_x) e_3, \quad x \in D,$$
(9)

where $e_3 = (0, 0, 1)^T$.

Lemma 2. With the notations given above let

$$\alpha = \min_{1 \le i \le n} x_i < \beta = \max_{1 \le i \le n} x_i.$$

Then

(a) φ is strictly increasing on $(-\infty, \alpha] \cap D$ and strictly decreasing on $[\beta, \infty) \cap D$. (b) φ has in D exactly one local minimum, say at $x = x_0$ and x_0 is in the interval (α, β) and is the only real root of

$$g(x) = a(x) + 2x b(x),$$
(10)

,

where

$$a(x) = (x + s_1)(x^2 + s_2) - (n + 1)(x^3 + s_3),$$

$$b(x) = (n + 1)(x^2 + s_2) - (x + s_1)^2.$$

Proof. Note first that if $M(d_x)$ is singular then $x = \alpha$ or $x = \beta$. This follows from $\alpha < \beta$ and the fact that $M(d_x)$ is regular iff $d_x = (x_1, x_2, \ldots, x_n, x)$ has at least three different components. To prove (a) let

$$h(x) = x^2 b(x) + x a(x) + c(x), \quad x \in \mathbb{R},$$

where

$$c(x) = (x+s_1)(x^3+s_3) - (x^2+s_2)^2,$$

$$F'(x) = \frac{d}{dx}F(x) = \begin{bmatrix} 0 & 1 & 2x \\ 1 & 2x & 3x^2 \\ 2x & 3x^2 & 4x^3 \end{bmatrix}, F''(x) = \frac{d^2}{dx^2}F(x) = \begin{bmatrix} 0 & 0 & 2 \\ 0 & 2 & 6x \\ 2 & 6x & 12x^2 \end{bmatrix}$$

and, for $x \in D$, $\delta(x) = \det M^{-2}(d_x)$. Then one obtains

$$\varphi'(x) = -e_3^T M^{-1}(d_x) F'(x) M^{-1}(d_x) e_3 = -2\delta(x) g(x) h(x), \quad x \in D,$$
(11)

and

$$\varphi^{\prime\prime}(x) = e_3^T M^{-1}(d_x) [2F^{\prime}(x)M^{-1}(d_x)F^{\prime}(x) - F^{\prime\prime}(x)]M^{-1}(d_x)e_3, \quad x \in D.$$
(12)

Putting $a = s_1 s_2 - n s_3$, $b = n s_2 - s_1^2$, $c = s_1 s_3 - s_2^2$, g(x) and h(x) can be written as

$$g(x) = \sum_{i=1}^{n} (x - x_i)^3 + 2bx + a = \sum_{i=1}^{n} (x - x_i)^3 + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (x_i - x_j)^2 (2x - x_i - x_j)$$
(13)

 $\quad \text{and} \quad$

$$h(x) = bx^{2} + ax + c = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (x_{i} - x_{j})^{2} (x - x_{i}) (x - x_{j}).$$
(14)

From this we see that

$$g(x)h(x) < 0$$
 for $x \in (-\infty, \alpha]$ and $g(x)h(x) > 0$ for $x \in [\beta, \infty)$.

Together with (11) this entails assertion (a), since $\delta(x) > 0$.

To prove (b) note first that

$$ng'(x) = 3(nx - s_1)^2 + (2n + 3)b > 0$$
 for all $x \in \mathbb{R}$.

Therefore, g(x) is strictly increasing and has exactly one real root x_0 . Also, from (13) one sees that $g(\alpha) < 0 < g(\beta)$; hence $x_0 \in (\alpha, \beta)$ and - noting the first remark in the proof $-x_0 \in D$. Further, from (12) one gets

$$\begin{aligned} \varphi''(x_0) &\geq -e_3^T M^{-1}(d_{x_0}) F''(x_0) M^{-1}(d_{x_0}) e_3 \\ &= a^2(x_0) - 4b(x_0)c(x_0) \\ &= (n+1)^{-2} [((n+1)a(x_0) + 2(x_0 + s_1)b(x_0))^2 + 4b^3(x_0)] > 0. \end{aligned}$$

Thus, at $x = x_0$ the function $\varphi(x)$ has a local minimum. It remains to show that there are no others. On referring to h(x) and from

$$n^{2}(a^{2} - 4bc) = (na + 2bs_{1})^{2} + 4b^{3} > 0$$

and (14) one sees that h(x) has two real roots, say x_1 and x_2 , $x_1 < x_2$. But $g(x) \cdot h(x)$ is a polynomial of degree 5 the highest coefficient of which is positive. Hence from (11) and $\delta(x) > 0$ it follows that the only local minimum of $\varphi(x)$ is at $x = x_0$.

Corollary 1. If d_{n+1}^* is an (n + 1)-point EMM-design on [-1, 1], then there exist $k, \ell, m \in \mathbb{N}, k + \ell + m = n + 1$, and $x \in (-1, 1)$ such that

$$d_{n+1}^* = \begin{bmatrix} -1 & x & 1 \\ k & m & \ell \end{bmatrix}.$$

Proof. Let $d_{n+1}^* = (x_1, x_2, \ldots, x_n, x_{n+1})$ and, without loss of generality, $x_{n+1} = \min_{1 \le i \le n+1} x_i$. If $x_{n+1} > -1$, then from part (a) of Lemma 2 one gets $\varphi(-1) < \varphi(x_{n+1})$. Thus, $d_{n+1} = (x_1, x_2, \ldots, x_n, -1)$ would be EMM-better than d_{n+1}^* . In the same way one sees that $\max_{1 \le i \le n+1} x_i = 1$.

Now let $i_0 \in \{1, 2, \ldots, n+1\}$ and $-1 < x_{i_0} < 1$; without loss of generality $i_0 = n + 1$. Since d_{n+1}^* is an EMM-design, for $d_x = (x_1, \ldots, x_n, x)$ one has

$$\varphi(x_{n+1}) = m^{33}(d_{n+1}^*) \le m^{33}(d_x) = \varphi(x)$$
 for all $x \in (-1, 1)$.

Thus at $x = x_{n+1}$ there is a local minimum of φ . From part (b) of Lemma 2 one gets

$$g(x_{n+1}) = a(x_{n+1}) + 2x_{n+1}b(x_{n+1}) = 0.$$

But a(x) and b(x) are constant on $\{x_1, x_2, \ldots, x_{n+1}\}$ and, therefore, $x_i = x_j$ for all i, j such that $-1 < x_i, x_j < 1$.

In view of Corollary 1 we can now restrict ourselves to designs of the form

$$d_{k,\ell,m,x} = \begin{bmatrix} -1 & x & 1 \\ k & m & \ell \end{bmatrix}, \quad x \in (-1,1), \quad k,\ell,m \in \mathbb{N}, \quad k+\ell+m=n.$$

For such designs one easily calculates

$$m^{33}(d_{k,\ell,m,x}) = [4k\ell + m(k+\ell) + 2(k-\ell)mx + (k+\ell)mx^2][4k\ell m(1-x^2)^2]^{-1}.$$
 (15)

We consider only the case n = 4p + 2, in the next lemma, with the exclusion $k + \ell \neq 2p + 1$.

Lemma 3. Let $k, \ell, m \in \mathbb{N}$, $k + \ell + m = 4p + 2$, $k + \ell \neq 2p + 1$, and $x \in (-1, 1)$. Then

$$m^{33}(d_{k,\ell,m,x}) > m^{33}(d_n^*).$$

Proof. From (2) we get

$$m^{33}(d_{k,\ell,m,x}) \ge n[m(k+\ell)(1-x^2)^2]^{-1} \ge n[m(k+\ell)]^{-1} \ge (2p+1)[2p(p+1)]^{-1}$$

and from (15) that

$$m^{33}(d_n^*) = [8p^2 + 8p + 1 - 2(2p+1)x_0 + (2p+1)^2x_0^2)][4p(p+1)(2p+1)(1-x_0^2)^2]^{-1}.$$

Applying $u(x_0) = 0$ twice, (cf. (6)) it is seen that

$$2p+1 > 2p(p+1)m^{33}(d_n^*)$$

is equivalent to

$$0 < 7(2p+1) - 2(52p^2 + 52p + 7)x_0 - (2p+1)(60p^2 + 60p - 7)x_0^2.$$
(16)

Because of $x_0 > 0$, (cf. Lemma 1.) (16) is equivalent to

$$x_0 < [(2p+1)(60p^2+60p-7)]^{-1}(\alpha - 52p^2 - 52p - 7) = x_1$$

where

$$\alpha = 2[2p(548p^3 + 1096p^2 + 667p + 119)]^{1/2} > 66p^2 + 66p + 7.$$

Hence

$$x_1 > 14p(p+1)[(2p+1)(60p^2+60p-7)]^{-1} \ge 7[30(2p+1)]^{-1} = x_2.$$

It is easy to show that $u(x_2) \ge 0 = u(x_0)$. Since u(x) is increasing, we get $x_0 \le x_2 < x_1$ which proves the assertion.

We are now prepared to prove Proposition 2: By the foregoing results, attention can be restricted to designs $d_{k,\ell,m,x}$, where $k + \ell = 2p + 1$ and $x \in (-1, 1)$, and – without loss of generality – $k < \ell$. In case $k = p, \ell = p + 1$, one gets

$$\psi(x) = m^{33}(d_{p,p+1,2p+1,x}) \ge m^{33}(d_n^*)$$

with equality holding iff $x = x_0$. This follows from the fact that $\psi(x)$ is strictly decreasing in $(-1, x_0]$ and strictly increasing in $[x_0, 1)$.

Now let $k and <math>x_1 \in (-1, 1)$ such that

$$m^{33}(d_{k,\ell,m,x_1}) = \min\{m^{33}(d_{k,\ell,m,x}): x \in (-1,1)\}.$$
(18)

Putting $j = \ell - k$ and, (cf. (10)), with $s_1 = j + (m-1)x_1$, $s_2 = m + (m-1)x_1^2$, $s_3 = j + (m-1)x_1^3$, $s_4 = m + (m-1)x_1^4$,

$$g(x_1) = m^2 x_1^3 - 3mj x_1^2 + (5m^2 - 2j^2)x_1 - mj,$$

it follows that (18) is, by Lemma 2, equivalent to $g(x_1) = 0$. Now it suffices to show that

$$m^{33}(d_{k,\ell,m,x_1}) > m^{33}(d_{p,p+1,2p+1,x_1}).$$
(19)

Because of $g(x_1) = 0$, (19) is equivalent to

$$m(j+1)x_1^2 - 2(m^2+j)x_1 + m(j+1) > 0,$$
(20)

and from

$$x_1 < 1 \le (m^2 + j)[m(j+1)]^{-1}$$

one gets the equivalence of (20) to

$$x_1 < [m^2 + j - ((m^2 - 1)(m^2 - j^2))^{1/2}][m(j+1)]^{-1} = x_2.$$
(21)

Since g is strictly increasing and $g(x_1) = 0$, (21) will hold true if one can show that $g(x_2) > 0$. Putting $z = m^2$, and after tedious calculations one finds that $g(x_2) > 0$ is equivalent to

$$(z-j^2)[2z^2+(5j+1)z+j(j^2+5j+2)] > (z-j^2)[2z+j^2+5j+2][(z-1)(z-j^2)]^{1/2}.$$
(22)

Because of $0 < j < z^{1/2}$, (22) is equivalent to

$$(3j4 + 14j3 + 24j2 + 18j + 5)z + j6 + 10j5 + 36j4 + 62j3 + 55j2 + 24j + 4 > 0.$$

Since the last inequality obviously holds true, Proposition 2 is proved.

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