



# Optimal designs for spline wavelet regression models

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## ABSTRACT

In this article we investigate the optimal design problem for some *wavelet regression* models. Wavelets are very flexible in modeling complex relations, and optimal designs are appealing as a means of increasing the experimental precision. In contrast to the designs for the Haar wavelet regression model (Herzberg and Traves 1994; Oyet and Wiens 2000), the *I*-optimal designs we construct are different from the *D*-optimal designs. We also obtain *c*-optimal designs. Optimal (*D*- and *I*-) *quadratic spline wavelet* designs are constructed, both analytically and numerically. A case study shows that a significant saving of resources may be realized by employing an optimal design. We also construct *model robust* designs, to address response misspecification arising from fitting an incomplete set of wavelets.

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## 1. Introduction and summary

Although their history dates back to the early 20th century (Haar, 1910), wavelets have been particularly popular in recent decades, both in theory and in applications. Applications of wavelets, in basic and biomedical sciences, can be found in the fields of signal processing, numerical analysis, and function representation, to mention only a few. See Chui (1992), Alpert (1992), Daubechies (1993), Antoniadis and Oppenheim (1995), Strang and Nguyen (1996) and Wojtaszczyk (1997) for more details. The use of wavelets in functional data analysis leads to applications in regression and subsequently in design theory—in a compact design space, one can use finitely many wavelet basis functions as regressors, to provide an adequate fit to the true response function. The wavelet model fitting becomes more precise as the order of the wavelets increases.

Since the 1950s, design theory for regression models has been developed extensively, in numerous papers. See, for example, Fedorov (1972), Dette and Studden (1997), Pukelsheim (1993), Atkinson et al. (2007) and references therein for detailed definitions, results and discussions.

We entertain an experimental setup in which, given inputs  $x_i$  chosen from a compact ‘design space’  $\mathcal{X}$ , the  $n$  outcomes  $Y_i$  depend on  $x_i$  via a regression model

$$Y_i = \sum_{j=0}^p \theta_j f_j(x_i) + \varepsilon_i, \quad i = 1, 2, \dots, n.$$

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Here  $\{f_j(x)\}_{j=0}^p$  are known functions,  $\boldsymbol{\theta} := (\theta_0, \theta_1, \dots, \theta_p)^T$  is a vector of unknown parameters, and the random errors  $\varepsilon_i$  are uncorrelated, with mean zero and variance  $\sigma^2$ . Given data  $\{(x_i, y_i)\}_{i=1}^n$ ,  $\boldsymbol{\theta}$  is estimated by the least squares estimate  $\hat{\boldsymbol{\theta}}$ . The design problem is to choose  $\{x_i\}_{i=1}^n$ , not necessarily distinct, in order to minimize some scalar function of the variance–covariance matrix  $\text{cov}[\hat{\boldsymbol{\theta}}]$ .

The exact experimental design  $\xi$  prescribes the number  $n\xi(x)$  of observations to be taken at a point  $x \in \mathcal{X}$ . Since the integer constraints typically make the exact design problem analytically intractable, we adopt the theory of *approximate design*, allowing  $\xi$  to be any probability measure supported on finitely many points in  $\mathcal{X}$ . Procedures to implement an approximate design  $\xi$  are discussed in Chapter 12 of Pukelsheim (1993). Intuitively, one makes  $\lfloor n\xi(x) \rfloor$  observations at  $x$  and then distributes the remaining resources in a prescribed manner—see our case study in Section 5.

Define  $\mathbf{f}(x) = (f_0(x), f_1(x), \dots, f_p(x))^T$ . The information matrix of a design  $\xi$  is

$$\mathbf{M}(\xi) = \int_{\mathcal{X}} \mathbf{f}(x) \mathbf{f}^T(x) d\xi,$$

and then  $\text{cov}[\hat{\boldsymbol{\theta}}] = (\sigma^2/n) \mathbf{M}^+(\xi)$ , where for definiteness we use the Moore–Penrose inverse  $\mathbf{M}^+$ . If  $\mathbf{c} \in \text{Range}(\mathbf{M}(\xi))$  we say that  $\mathbf{c}^T \boldsymbol{\theta}$  is *estimable*, and then the *c-optimal* design is that which minimizes  $\mathbf{c}^T \mathbf{M}^+(\xi) \mathbf{c}$ . When  $\mathbf{M}(\xi)$  is non-singular, which we shall assume except when discussing *c*-optimality,  $\mathbf{M}^+ = \mathbf{M}^{-1}$  and we can define optimality criteria through scalar functions of  $\mathbf{M}^{-1}(\xi)$ , as follows. Define  $d(x, \xi) = \mathbf{f}^T(x) \mathbf{M}^{-1}(\xi) \mathbf{f}(x)$ ; note that the variance of the estimate  $\mathbf{f}^T(x) \hat{\boldsymbol{\theta}}$  of  $E[Y|x]$  is proportional to  $d(x, \xi)$ , with the constant  $\sigma^2/n$  of proportionality being independent of the design. A design  $\xi$  is called *D*-optimal, *A*-optimal, *E*-optimal, *G*-optimal or *I*-optimal if it minimizes  $|\mathbf{M}^{-1}(\xi)|$ ,  $\text{trace}(\mathbf{M}^{-1}(\xi))$ ,  $\lambda_{\max}(\mathbf{M}^{-1}(\xi))$  (the largest eigenvalue),  $\max_{x \in \mathcal{X}} d(x, \xi)$  or  $\int_{\mathcal{X}} d(x, \xi) dx$ , respectively.

In Section 3 we construct optimal designs for those wavelet regression models developed in Section 2. When  $\mathbf{f}(x)$  is a vector of Haar wavelets, Herzberg and Traves (1994) obtained the *D*-optimal design. Oyet and Wiens (2000) show that this design is also *A*-optimal and *I*-optimal. Xie and Li (unpublished) find the *D*-optimal design for piecewise linear spline wavelet regression. In this article, we show that this design, given by Xie and Li, is *A*- and *E*-optimal but not *I*-optimal. We construct the *I*-optimal and *c*-optimal designs. The latter case includes optimal designs for interpolation and extrapolation. Since  $\mathbf{f}(x)$  is no longer a Chebyshev system, one can view the *c*-optimality as a partial extension of Studden (1968).

We also obtain results for the quadratic spline wavelet model. The mathematical complexity restricts us to some simple cases, and so in Section 4 we discuss the numerical construction of these designs. We exhibit these in several cases which are apparently not yet in the literature. Then in Section 5 we test these designs on simulated data based on an experiment in automotive engineering, with a response function which is difficult to model in a more conventional way. We finish with a discussion of *model robustness* of design; again algorithms are given leading to the construction of both approximate and exact designs.

The usefulness of wavelet methods in regression arises from the ability of linear combinations of wavelets to approximate arbitrarily closely any response function which is square integrable over the design space. Of course Fourier expansions yield this property as well, and depending on the complexity of the response function such an expansion might lead to a more economical representation, especially when the response is periodic. There is a substantial literature on design for such *trigonometric regression* models, well-reviewed by Dette et al. (2011). The situation is somewhat similar to that of design for quadratic spline wavelet regression as discussed in this article—except for quite simple models analytic results are sparse, but there are theorems allowing one to check whether or not a particular design is optimal. The numerical methods we discuss in Sections 4 and 5 are as applicable to trigonometric models as to wavelet models.

The designs presented here are constructed via computations implemented in MATLAB; the code is available from us.

## 2. Preliminaries

We use notation and definitions as in Wojtaszczyk (1997) and begin with the representation of the space  $\mathcal{L}^2(\mathcal{R})$  of square integrable functions on  $\mathcal{R}$  as the union of an increasing sequence of closed sets of functions:

$$\mathcal{L}^2(\mathcal{R}) = \cup_{r \in \mathbb{Z}} V_r, \dots \subset V_{-2} \subset V_{-1} \subset V_0 \subset V_1 \subset V_2 \subset \dots$$

The sets  $V_r$  are dilates of one another, in that  $f(x) \in V_r$  iff  $f(2^{-r}x) \in V_0$ , the set  $V_0$  is closed under integer translations:

$$f(x) \in V_0 \Leftrightarrow f(x - k) \in V_0 \quad \forall k \in \mathbb{Z} = \{0, \pm 1, \pm 2, \dots\},$$

(i.e.  $f(x) = f(x - [x])$ ) and there exists a *scaling function* (also known as a *father wavelet*)  $\phi \in V_0$  whose integer translates span  $V_0$ . The functions  $\phi_{r,k}(x) = 2^{r/2} \phi(2^r x - k)$ , for  $k \in \mathbb{Z}$ , form an orthonormal basis for  $V_r$ , which we shall call the *natural basis*. Through a *multiresolution analysis* the space  $V_r$  can be represented as the direct sum of mutually orthogonal subspaces  $V_r = V_0 \oplus \bigoplus_{l=0}^{r-1} W_l$ , where  $W_l$  is the orthogonal complement of  $V_l$  in  $V_{l+1}$ . An orthonormal basis of  $W_l$  is  $\{\psi_{l,k}(x) = 2^{l/2} \psi(2^l x - k)\}$  for a suitably constructed *mother wavelet*  $\psi$ . An alternate, orthonormal *wavelet basis* for  $V_r$  is then given by the union of these bases for  $\{V_0, W_l : l = 0, \dots, r-1\}$ .

We are concerned here with the approximation of a regression response  $E[Y|x] \in \mathcal{L}^2[0, 1]$ . We restrict to wavelet classes for which the restriction  $V_0[0, 1]$  of the members of  $V_0$  to  $\mathcal{X} = [0, 1]$  is finite dimensional, by virtue of satisfying the conditions of the following lemma due to Wojtaszczyk (1997). Since it is not proved there we give a proof in the Appendix.

**Lemma 1.** Suppose that  $V_0$  contains a function  $\gamma(x)$  vanishing off of  $[K_1, K_2]$  for integers  $K_1, K_2$  and is such that:

(A1) the set  $\{\gamma(x - k) \mid k \in \mathbb{Z}\}$  is a basis for  $V_0$ ;

(A2) the set  $\{\gamma(x - k)I_{[0,1]}(x) \mid k \in \mathcal{K}_0\}$ , where  $\mathcal{K}_0 := \{-K_2 + 1, \dots, -K_1\}$ , is linearly independent.

Then:

- (i) the set  $\{\gamma(x - k)I_{[0,1]}(x) \mid k \in \mathcal{K}_0\}$  is a basis for  $V_0[0, 1]$ ;
- (ii) a basis for  $V_r[0, 1]$  is the set  $\mathcal{V}_r := \{2^{r/2}\gamma(2^r x - k)I_{[0,1]}(x) \mid k \in \mathcal{K}_r\}$ , where

$$\mathcal{K}_r := \{i + j \mid i = 0, \dots, 2^r - 1, j \in \mathcal{K}_0\} = \{-K_2 + 1, \dots, -K_1 + 2^r - 1\};$$

- (iii) there is a set  $\mathcal{K}_r^* \subset \mathbb{Z}$ , with the same cardinality  $p_r := K_2 - K_1 + 2^r - 1$  as  $\mathcal{K}_r$ , such that a basis for  $V_r[0, 1]$  is

$$\mathcal{V}_r^* := \{v_{r,k}(x) = \phi_{r,k}(x)I_{[0,1]}(x) \mid k \in \mathcal{K}_r^*\}.$$

We shall refer to the basis in (iii) of Lemma 1 as the natural basis for  $V_r[0, 1]$ . In a similar manner the elements of a wavelet basis for  $V_r$  may be restricted to form a wavelet basis for  $V_r[0, 1]$ . There will of course be other bases as well. If the vectors  $\mathbf{v}(x)$  and  $\mathbf{w}(x)$  consist of the elements of two bases, then there is a linear relationship between them:  $\mathbf{v}(x) = \mathbf{P}\mathbf{w}(x)$  for a nonsingular matrix  $\mathbf{P}$ .

**Example 2.1** (Haar Wavelets). Here the scaling function is  $\phi(x) = I_{[0,1]}(x)$  and  $V_r[0, 1]$  consists of those functions which are constant on all sub-intervals  $[2^{-r}k, 2^{-r}(k+1)]$ ,  $k = 0, \dots, 2^r - 1$ . Lemma 1 holds with  $K_1 = 0$ ,  $K_2 = 1$ ,  $\gamma = \phi$ . A wavelet basis is determined from  $\phi(x)$  and the mother wavelet  $\psi(x) = I_{[0,1/2)}(x) - I_{[1/2,1)}(x)$ ; see Chapter 1 of Wojtaszczyk (1997) for details.

**Example 2.2** (Spline Wavelets). Let  $S_d$  be the space of all splines of order  $d$  with integer nodes, so that if  $f \in S_d$  then  $f \in C^{d-1}$  and is a polynomial of degree at most  $d$  within each interval  $[k, k+1]$ . This space has as a (Riesz) basis the translates  $\{N_d(x - k) \mid k = -d, \dots, 0\}$  of the B-splines  $N_d(x)$  defined recursively by  $N_0(x) = I_{[0,1]}(x)$ , and (with  $*$  denoting convolution),  $N_d(x) = N_{d-1}(x) * N_0(x)$ . The support of  $N_d(x)$  is  $[0, d+1]$ ; in the interior of this interval  $N_d(x)$  is strictly positive. Thus (A1) of Lemma 1 holds with  $K_1 = 0$ ,  $K_2 = d+1$ ,  $\gamma = N_d$ . An induction on  $d$  combined with the identity  $N'_d(x) = N_{d-1}(x) - N_{d-1}(x-1)$  shows that (A2) holds as well. Note that when  $d = 0$  the spline wavelets coincide with the Haar wavelets and  $N_0(x)$  is the scaling function. For  $d > 0$  the scaling function and mother wavelet are substantially more complicated; this need not concern us here since the basis given above is the most convenient one for our purposes. Xie (unpublished) combines a wavelet basis for  $\bigoplus_{l=0}^{n-1} W_l[0, 1]$  with the basis of Lemma 1(i) to obtain a regression model. The father wavelet for the  $d = 1$  spline wavelet (linear spline wavelet) is

$$\phi(x) = N_1(x) = xI_{[0,1)}(x) + (-x+2)I_{[1,2]}(x), \quad (1)$$

with support  $[0, 2]$ . Similarly, the father wavelet for the quadratic spline wavelet ( $d = 2$ ) is

$$\phi(x) = N_2(x) = \frac{x^2}{2}I_{[0,1)}(x) + \left(-x^2 + 3x - \frac{3}{2}\right)I_{[1,2)}(x) + \left(\frac{x^2}{2} - 3x + \frac{9}{2}\right)I_{[2,3]}(x), \quad (2)$$

with support  $[0, 3]$ .

Now, the regression model we consider is

$$E[Y|x] = \mathbf{f}^T(x)\boldsymbol{\theta} = \sum_{k=0}^{p_r-1} \theta_k f_k(x), \quad x \in [0, 1], \quad (3)$$

with  $\mathbf{f}(x)$  consisting of the  $p_r$  elements of  $\mathcal{V}_r^*$ .

It is well known that in this framework  $D$ -optimality is equivalent to  $G$ -optimality, and that  $D$ -,  $G$ - and  $I$ -optimal designs are invariant under reparameterizations  $\mathbf{f}^T(x) \mapsto \mathbf{f}^T(x)\mathbf{P}^{-1}$ ,  $\boldsymbol{\theta} \mapsto \mathbf{P}\boldsymbol{\theta}$  that leave the mean response unchanged. However  $A$ - and  $E$ -optimal designs do not have this property of invariance. As to  $c$ -optimality, it is invariant when  $\mathbf{c}$  is of the form  $\mathbf{f}(x_0)$ , corresponding to interpolation when  $x_0 \in [0, 1]$  and to extrapolation when  $x_0 \notin [0, 1]$ .

### 3. Optimal designs

#### 3.1. Linear spline wavelet regression model

We use the linear spline wavelets determined by (1) to define the regressors in the regression model (3) with design space  $\mathcal{X} = [0, 1]$ . Thus for a chosen non-negative integer  $r$ ,

$$f_k(x) = \phi(2^r x - k + 1) \quad (4)$$

where  $k = 0, 1, \dots, p_r - 1 = 2^r$ . Xie and Li (unpublished) show that the equispaced design

$$\xi_D = \frac{1}{2^r + 1} \sum_{i=0}^{2^r} \delta_{\left\{\frac{i}{2^r}\right\}},$$

is  $D$ -optimal, with corresponding information matrix  $\mathbf{M}(\xi_D) = \frac{1}{2^r + 1} \mathbf{I}$ , by verifying that  $\max_{x \in [0, 1]} d(x, \xi_D) = 2^r + 1$ —this is the necessary and sufficient condition for optimality, from the celebrated Kiefer and Wolfowitz (1960) theorem.

In Theorems 1 and 2 we also invoke the Kiefer–Wolfowitz Theorem, by which a design  $\xi_0$  is  $A$ - or  $I$ -optimal iff, for any design  $\xi_1$ , we have

$$\text{tr}(\mathbf{M}^{-1}(\xi_0)\mathbf{H}) - \text{tr}(\mathbf{M}^{-1}(\xi_0)\mathbf{M}(\xi_1)\mathbf{M}^{-1}(\xi_0)\mathbf{H}) \geq 0, \quad (5)$$

where  $\mathbf{H} = \mathbf{I}$  in the case of  $A$ -optimality and  $\mathbf{H} = \int_0^1 \mathbf{f}(x)\mathbf{f}^T(x)dx$  in the case of  $I$ -optimality. See, e.g., Pukelsheim (1993).

**Theorem 1.** The design  $\xi_D$  is also  $A$ - and  $E$ -optimal for the regression model (3), in which the regressors are defined by (4) with  $\phi(x)$  given by (1).

**Proof.** For  $A$ -optimality, with  $\xi_0 = \xi_D$ ,  $\mathbf{M}(\xi_0) = \frac{1}{2^r + 1} \mathbf{I}_{2^r + 1}$  and  $\mathbf{H} = \mathbf{I}_{2^r + 1}$  in (5) we obtain the condition  $\text{tr}(\mathbf{M}(\xi_1)) \leq 1$ , verified as follows:

$$\begin{aligned} \text{tr}(\mathbf{M}(\xi_1)) &= \int_0^1 \mathbf{f}^T(x)\mathbf{f}(x)d\xi_1 = \sum_{k=0}^{2^r} \int_{\frac{k}{2^r}}^{\frac{k+1}{2^r}} [(2^r x - k)^2 + (1 + k - 2^r x)^2] d\xi_1 \\ &\leq (2^r + 1)^{-2} \text{tr}(\mathbf{M}^{-1}(\xi_0)) = 1. \end{aligned}$$

For the  $E$ -optimality, since  $\lambda_{\min}(\mathbf{M}(\xi_D)) = 1/(2^r + 1)$ , with the corresponding eigenvectors being the columns  $\{e_k\}_{k=0}^{2^r}$  of  $\mathbf{I}_{2^r + 1}$ , we have the following. With  $w_k = 1/(2^r + 1)$ ,

$$\mathbf{f}^T(x)(e_0, \dots, e_{2^r}) \text{diag}(w_0, \dots, w_{2^r})(e_0, \dots, e_{2^r})^T \mathbf{f}(x) = \frac{1}{2^r + 1} \sum_{k=0}^{2^r} f_k^2(x) \leq \frac{1}{2^r + 1},$$

for all  $x \in [0, 1]$ , with equality at the support points of  $\xi_D$ . Thus, by Theorem 2.1 in Dette and Grigoriev (2014),  $\xi_D$  is  $E$ -optimal. ■

We comment that  $A$ -optimality can also be proved by using Theorem 2.11.1 of Fedorov (1972). A consequence of the following theorem is that  $\xi_D$  is not  $I$ -optimal.

**Theorem 2.** The  $I$ -optimal design for the linear spline wavelet regression is

$$\xi_I = a(\delta_{\{0\}} + \delta_{\{1\}}) + b \sum_{k=1}^{2^r-1} \delta_{\left\{\frac{k}{2^r}\right\}},$$

where  $a = 1/(\sqrt{2}(2^r - 1 + \sqrt{2}))$  and  $b = \sqrt{2}a$ .

**Proof.** We proceed as in the proof of Theorem 1, but with  $\xi_0 = \xi_I$  and

$$\mathbf{H} = \int_0^1 \mathbf{f}(x)\mathbf{f}^T(x)dx = \frac{1}{2^r 6} \begin{pmatrix} 2 & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & 4 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & 4 & 1 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & 1 & 4 & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & 2 \end{pmatrix},$$

so that  $\mathbf{M}(\xi_0) = \text{diag}(a, b, \dots, b, a)$ . Then

$$\text{tr}(\mathbf{M}^{-1}(\xi_0)\mathbf{H}) = \frac{1}{2^r 6} \left[ \frac{2}{a} + \frac{4}{b}(2^r - 1) + \frac{2}{a} \right] = \frac{2(2^r - 1 + \sqrt{2})^2}{2^r 3},$$

and

$$\begin{aligned}
 \text{tr}(\mathbf{M}^{-1}(\xi_0)\mathbf{M}(\xi_1)\mathbf{M}^{-1}(\xi_0)\mathbf{H}) &= \int_0^1 \mathbf{f}^T(x)\mathbf{M}^{-1}(\xi_0)\mathbf{H}\mathbf{M}^{-1}(\xi_0)\mathbf{f}(x)d\xi_1 \\
 &= \frac{1}{2^r 6} \int_0^1 \left( \frac{2}{a^2} (1-2^r x)^2 I_{\left[0, \frac{1}{2^r}\right]}(x) + \frac{4}{b^2} \sum_{k=1}^{2^r-1} \left[ (2^r x - k + 1)^2 I_{\left[\frac{k-1}{2^r}, \frac{k}{2^r}\right]}(x) \right. \right. \\
 &\quad \left. \left. + (k+1-2^r x)^2 I_{\left[\frac{k}{2^r}, \frac{k+1}{2^r}\right]}(x) \right] + \frac{2}{a^2} (2^r x - 2^r + 1)^2 I_{\left[\frac{2^r-1}{2^r}, 1\right]}(x) \right. \\
 &\quad \left. + \frac{2}{ab} (1-2^r x)(2^r x) I_{\left[0, \frac{1}{2^r}\right]}(x) + \frac{2}{b^2} \sum_{k=1}^{2^r-1} (k+1-2^r x)(2^r x - k) I_{\left[\frac{k}{2^r}, \frac{k+1}{2^r}\right]}(x) \right. \\
 &\quad \left. + \frac{2}{ab} (2^r - 2^r x)(2^r x - 2^r + 1) I_{\left[\frac{2^r-1}{2^r}, 1\right]}(x) \right) d\xi_1 \\
 &\leq \frac{1}{2^r 6} \frac{2}{a^2} = \frac{2(2^r - 1 + \sqrt{2})^2}{2^r 3};
 \end{aligned}$$

now (5) follows. ■

We have obtained the  $c$ -optimal designs under the condition that the signs of the elements of  $\mathbf{c}$  be either constant or alternating. Define

$$S_1 = \{\mathbf{c} : \text{all } c_k \geq 0, \text{ or all } c_k \leq 0\},$$

$$S_2 = \{\mathbf{c} : \text{all } (-1)^k c_k \geq 0, \text{ or all } (-1)^k c_k \leq 0\}.$$

The proof of the following theorem depends on Elfving's Theorem (Elfving, 1952) and Lemma 2.1 of Studden (1968). For the readers' convenience, we state these two theorems in the Appendix.

**Theorem 3.** For any  $\mathbf{c} \in S_1 \cup S_2$  for which  $\mathbf{c}^T \boldsymbol{\theta}$  is estimable, the design  $\xi_c$ , with support points  $\{2^{-r}k\}_{k=0}^{2^r}$  and corresponding weights

$$w_k = \frac{|c_k|}{\sum_{l=0}^{2^r} |c_l|}, \quad k = 0, 1, \dots, 2^r,$$

is  $c$ -optimal.

**Proof.** For any vector  $\mathbf{c}$ , we have  $\mathbf{c} = \sum_{k=0}^{2^r} c_k \mathbf{f}(k/2^r) = \sum_{k=0}^{2^r} \text{sign}(c_k) |c_k| \mathbf{f}(k/2^r)$ . Let  $\beta = (\sum_{l=0}^{2^r} |c_l|)^{-1}$ , then  $\beta \mathbf{c} = \sum_{k=0}^{2^r} \text{sign}(c_k) w_k \mathbf{f}(k/2^r)$ , which implies that  $\beta \mathbf{c} \in V$ , defined in Elfving's Theorem in the Appendix. Here, we set  $\text{sign}(c_k) = 1$  or  $-1$  if  $c_k = 0$ .

If  $\mathbf{c} \in S_2$ , without loss of generality, we assume  $(-1)^k \text{sign}(c_k) = 1$ ,  $k = 0, 1, \dots, 2^r$ . Define a function  $e(x) := \sum_{k=0}^{2^r} (-1)^k f_k(x)$ , then  $e(2^{-r}k) = (-1)^k$ ,  $k = 0, 1, \dots, 2^r$  and  $|e(x)| \leq 1$ . By applying  $e(x)$  to Lemma 2.1 of Studden (1968), we can show that  $\beta \mathbf{c}$  is a boundary point of  $V$ . If  $\mathbf{c} \in S_1$ , by applying the function  $U(x) := \sum_{k=0}^{2^r} f_k(x) \equiv 1$  to the same lemma, we show that  $\beta \mathbf{c}$  is a boundary point of  $V$ . Thus, by Elfving's Theorem,  $\xi_c$  is  $c$ -optimal if  $\mathbf{c} \in S_1 \cup S_2$ . ■

As examples, if  $\mathbf{c} = (1, 1, \dots, 1)^T$ , then  $\mathbf{c} \in S_1$ , and  $\xi_c$  coincides with  $\xi_D$ . If we want to compare the average of odd-order coefficients and the average of even-order coefficients, that is,  $\mathbf{c} = \left(-\frac{1}{2^{r-1}+1}, \frac{1}{2^{r-1}}, -\frac{1}{2^{r-1}+1}, \dots, \frac{1}{2^{r-1}}, -\frac{1}{2^{r-1}+1}\right)^T$ , then  $\mathbf{c} \in S_2$ , and  $\xi_c$  has weight  $\frac{1}{2^{r+2}}$  on design points  $\frac{2k}{2^r}$ , where  $k = 0, 1, \dots, 2^{r-1}$ , and weight  $\frac{1}{2^r}$  on design points  $\frac{2k+1}{2^r}$ , where  $k = 0, 1, \dots, 2^{r-1} - 1$ . Note that, for  $\mathbf{c}_t = \mathbf{f}(t)$ ,  $t \in [2^{-r}k, 2^{-r}(k+1)]$ , the optimal interpolation design  $\xi_{c_t}$  has only two support points  $2^{-r}k$  and  $2^{-r}(k+1)$ , with weights  $f_k(t)/(f_k(t) + f_{k+1}(t))$  and  $f_{k+1}(t)/(f_k(t) + f_{k+1}(t))$  separately. This is a singular design. For  $\mathbf{c} \notin S_1 \cup S_2$ , we have not found  $c$ -optimal designs, partly because for such  $\mathbf{c}$ , the union of non-empty domains of the regressors corresponding to one sign (+ or −) is only a subset of  $[0, 1]$ .

### 3.2. Quadratic spline wavelet regression model

When using the quadratic spline wavelet (2) to define the wavelet regression model (3) of order  $r$ , the number of regressors is, from Lemma 1(iii),  $p_r = 3 - 0 + 2^r - 1 = 2^r + 2$ . The model is more complicated than the linear spline model in that each regressor is quadratic, and in the linear spline model there is only one regressor having a non-zero value (actually maximum value) at each of the points  $\{k/2^r\}_{k=0}^{2^r}$ . This makes it difficult to construct the optimal designs. We only have analytic results for  $r \in \{0, 1\}$ ; in Section 4 we discuss numerical approaches.

**Theorem 4.** For the wavelet regression model (3) of order  $r$ , with regressors defined by the father wavelet (2), we have

- (i) when  $r = 0$ , the mean response has three parameters and the  $D$ -optimal design  $\xi_D$  puts equal weight on  $0, \frac{1}{2}, 1$ ;
- (ii) when  $r = 1$ , the mean response has four parameters and the  $D$ -optimal design  $\xi_D$  puts equal weight on  $0, \frac{9-\sqrt{17}}{16}, \frac{7+\sqrt{17}}{16}, 1$ .

**Proof.** We give the proof of (ii); that of (i) – which is somewhat well-known – is similar but simpler. After some algebra, we find that the information matrix  $\mathbf{M}(\xi_D)$  is of the form  $(1/4096) (\mathbf{M}_1 + \sqrt{17}\mathbf{M}_2)$ , with

$$\mathbf{M}_1 = \begin{pmatrix} 561 & 454 & 297 & 0 \\ * & 3269 & -1236 & 297 \\ * & * & 3269 & 454 \\ * & * & * & 561 \end{pmatrix}, \quad \mathbf{M}_2 = \begin{pmatrix} -9 & 42 & -65 & 0 \\ * & -381 & 436 & -65 \\ * & * & -381 & 42 \\ * & * & * & -9 \end{pmatrix}.$$

The variance function  $d(x, \xi_D) = \mathbf{f}^T(x) \mathbf{M}^{-1}(\xi_D) \mathbf{f}(x)$  is

$$d(x, \xi_D) = (ax^4 + bx^3 + cx^2 + dx + e) I_{[0, 1/2)}(x) + (fx^4 + gx^3 + hx^2 + ix + j) I_{[1/2, 1]}(x),$$

in which the coefficients are

Coefficient	Value	Coefficient	Value
$a$	$125\sqrt{17}/2 + 965/2$	$f$	$125\sqrt{17}/2 + 965/2$
$b$	$-(55\sqrt{17} + 655)$	$g$	$-(195\sqrt{17} + 1275)$
$c$	$10\sqrt{17} + 290$	$h$	$220\sqrt{17} + 1220$
$d$	$-40$	$i$	$-(105\sqrt{17} + 505)$
$e$	$4$	$j$	$35\sqrt{17}/2 + 163/2$

Now, it can be shown that in  $(0, 1)$ , the function  $d(x, \xi_D)$  has the stationary points  $\left\{ \frac{41-\sqrt{17}}{416}, \frac{9-\sqrt{17}}{16}, \frac{1}{2}, \frac{7+\sqrt{17}}{16}, \frac{375+\sqrt{17}}{416} \right\}$ . Furthermore, by checking the second derivative of  $d(x, \xi_D)$ , we obtain the local minima at  $\frac{41-\sqrt{17}}{416}, \frac{1}{2}$ , and  $\frac{375+\sqrt{17}}{416}$ , and local maxima at  $\frac{9-\sqrt{17}}{16}$  and  $\frac{7+\sqrt{17}}{16}$ . These and the fact that  $d(0, \xi_D) = d\left(\frac{9-\sqrt{17}}{16}, \xi_D\right) = d\left(\frac{7+\sqrt{17}}{16}, \xi_D\right) = d(1, \xi_D) = 4$  imply that  $d(x, \xi_D) \leq 4, x \in [0, 1]$ , with equality being held at the support points of  $\xi_D$ . By the Kiefer–Wolfowitz Theorem, we conclude that  $\xi_D$  is a  $D$ -optimal design for the quadratic spline wavelet regression model of order  $r = 1$ . This completes the proof. ■

**Remark.** Optimal design for spline regression has been considered by Kaishev (1989) and Heiligers (1999), and part (ii) of Theorem 4 can also be derived from the Lemma of Kaishev (1989, p. 43). We present it as above partly to motivate our numerical treatment, for  $r > 1$ , in the next section.

#### 4. Numerical construction of quadratic spline wavelet designs

We have derived and implemented algorithms for the construction of  $D$ - and  $I$ -optimal designs for quadratic spline wavelets. For this, we first discretize the design space as  $\chi = \{x_i = \frac{i-1}{N-1}; i = 1, \dots, N\}$ , with  $N = 1001$  for a close approximation to a continuous interval.

Let  $\mathbf{F}_{N \times p_r}$  have rows  $\{\mathbf{f}^T(x_i); i = 1, \dots, N\}$  and for a design  $\xi$  let  $\mathbf{D}(\xi)$  be the diagonal matrix with diagonal  $\{\xi(x_1), \dots, \xi(x_N)\}$ . It is convenient to work in a canonical form. Let  $\mathbf{Q}_{N \times p_r}$  be such that its columns form an orthogonal basis for the column space of  $\mathbf{F}$ —this is ‘ $\mathbf{Q}$ ’ in the QR-decomposition of  $\mathbf{F}$ . Define  $\mathbf{R}(\xi) = \mathbf{Q}^T \mathbf{D}(\xi) \mathbf{Q}$ . Then the  $D$ - and (scaled)  $I$ -criteria to be minimized are, respectively,

$$\mathcal{D}_\xi = |\mathbf{M}^{-1}(\xi)|^{1/p_r} = |\mathbf{R}^{-1}(\xi)|^{1/p_r},$$

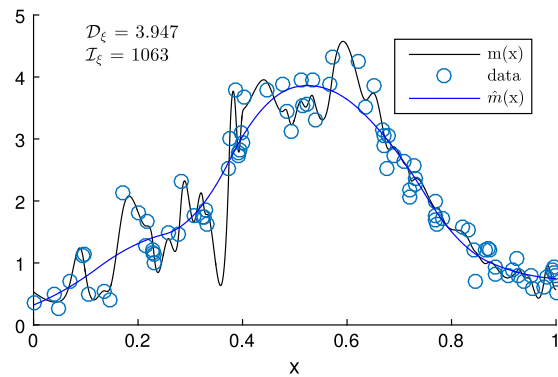
$$\mathcal{I}_\xi = \text{tr} \mathbf{F} \mathbf{M}^{-1}(\xi) \mathbf{F}^T / p_r = \text{tr} \mathbf{R}^{-1}(\xi) / p_r.$$

Denote by  $\{\mathbf{q}_i^T; i = 1, \dots, N\}$  the rows of  $\mathbf{Q}$ . As in the Kiefer–Wolfowitz Theorem, the necessary and sufficient conditions for the optimality of a design  $\xi^0$  are

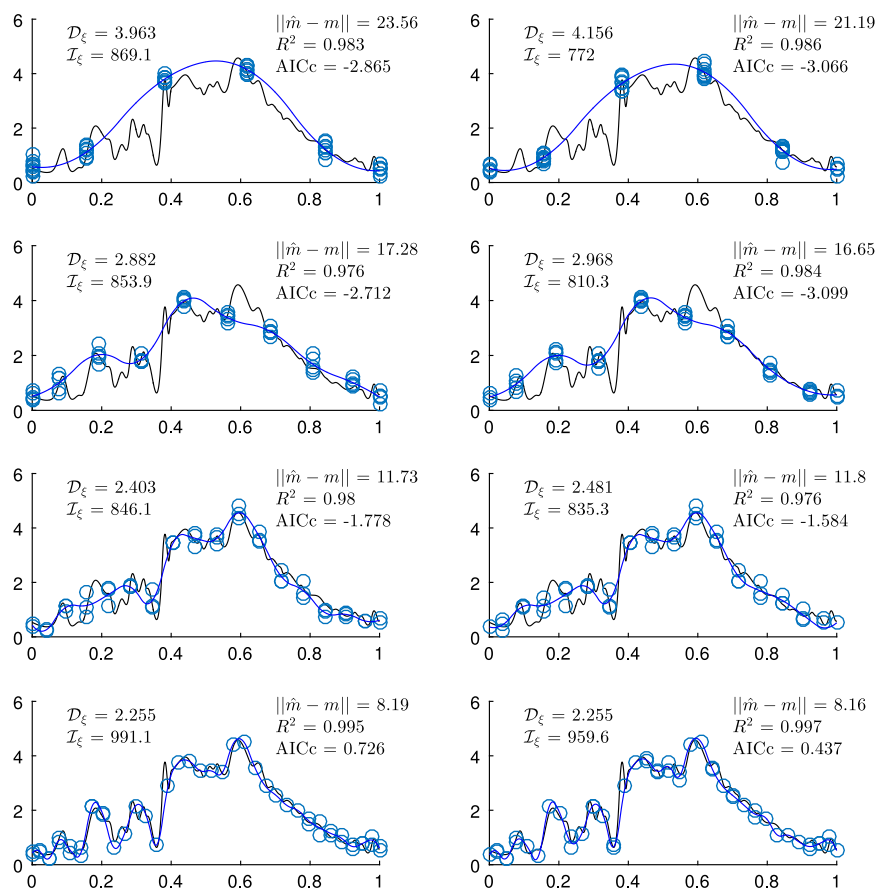
$D$ -criterion:  $\mathbf{q}_i^T \mathbf{R}^{-1}(\xi^0) \mathbf{q}_i - p_r \leq 0$  for all  $i = 1, \dots, N$ , with equality if  $\xi_i^0 > 0$ ;

$I$ -criterion:  $\mathbf{q}_i^T \mathbf{R}^{-2}(\xi^0) \mathbf{q}_i - \text{tr} \mathbf{R}^{-1}(\xi^0) \leq 0$  for all  $i = 1, \dots, N$ , with equality if  $\xi_i^0 > 0$ .





**Fig. 2.** Response  $m(x)$  created by smoothing the [Brinkman \(1981\)](#) data; simulated data at Brinkman design points; fitted quadratic wavelet ( $r = 3$ ) response  $\hat{m}(x)$ .



**Fig. 3.** Implementations of  $D$ - (left panel) and  $I$ - (right panel) optimal designs for quadratic spline wavelet models of orders  $r = 2$  (top) to  $r = 5$  (bottom). Legend as in [Fig. 2](#).

correction). [Rafałłowicz and Schwabe \(2003\)](#) employ a similar residual-based criterion in their study of equally spaced designs in nonparametric regression.

We have constructed and implemented a variety of  $D$ - and  $I$ -optimal designs for quadratic spline wavelets, using each of  $r = 1, \dots, 5$  and simulated data as described above. In all cases we used a design size of  $n = 50$ ; this called for some replications and so the frequencies used were determined by applying the ‘efficient design apportionment’ method of [Pukelsheim and Rieder \(1992\)](#). See [Fig. 3](#). We have not plotted the results for  $r = 1$  since the fits were so poor. The AICc criterion picks  $r = 2$  for the  $D$ -optimal design and  $r = 3$  for the  $I$ -optimal design. In each case a substantially better fit is

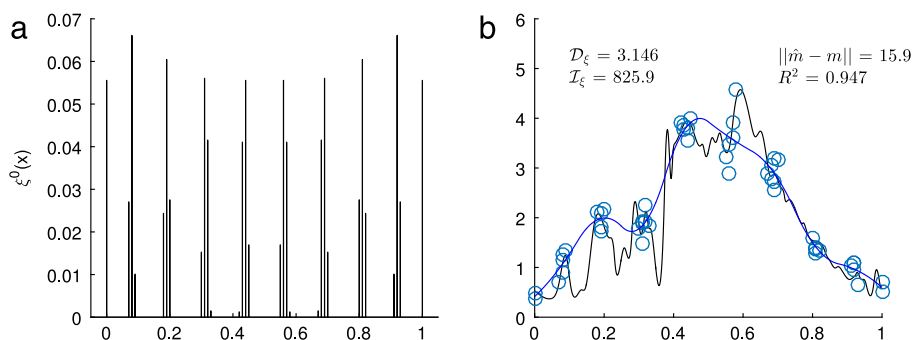


Fig. 4. (a)  $I$ -robust design for order  $r = 3$  quadratic spline wavelet models. (b) Implementation of this design as with those of Fig. 1.

obtained by using larger values of  $r$ . This is borne out by the values of

$$\|\hat{m} - m\| = \left( \sum_{x \in \mathcal{X}} (\hat{m}(x) - m(x))^2 \right)^{1/2};$$

these would of course not be available to the experimenter.

### 5.1. Robustness considerations

As in Section 2, the wavelets which form the regressors constitute only the first few terms of a series expansion converging to a given response function in  $\mathcal{L}^2[0, 1]$ . A natural problem is then that of designing in such a way as to control a measure of the mean squared error, rather than merely the variation, in the face of biases arising from fitting an insufficient collection of wavelets. We address this problem in the following way. We write the mean response as  $E[Y|x] = \mathbf{f}^T(x)\boldsymbol{\theta} + \psi(x)$ , where  $\mathbf{f}$  contains the wavelets employed in the experimenter's intended model,  $\boldsymbol{\theta} := \arg \min_{\boldsymbol{\eta}} \int_{\mathcal{X}} (E[Y|x] - \mathbf{f}^T(x)\boldsymbol{\eta})^2 dx$ , and  $\psi(x) := E[Y|x] - \mathbf{f}^T(x)\boldsymbol{\theta}$  is 'model error', orthogonal to  $\mathbf{f}(x)$  and bounded in  $\mathcal{L}^2(\mathcal{X})$ . Thus  $\psi$  is representable as a series in those wavelets not being fitted. For a constant  $\tau \geq 0$  we impose a bound of  $\tau/\sqrt{n}$  on the  $\mathcal{L}^2$  norm of  $\psi$ ; this ensures that the contribution of (squared) bias to the mean squared error drops at the same rate as that of variation. We adopt a *minimax* approach, and define the  $D$ -robust (respectively,  $I$ -robust) design problem as that of finding a design so as to minimize, respectively,

$$\mathcal{D}_{\max}(\xi) = \max_{\psi} \left( \det E \left[ (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})^T \right] \right)^{1/p},$$

$$\mathcal{I}_{\max}(\xi) = \max_{\psi} \int_{\mathcal{X}} E \left[ \left( \mathbf{f}^T(x)\hat{\boldsymbol{\theta}} - E[Y|x] \right)^2 \right] dx.$$

See Wiens (2015) for the general theory of such problems in model robustness of design, and Oyet and Wiens (2000) for solutions in *multiwavelet* models.

Here we apply the algorithms developed in Wiens (submitted for publication), employed above in the  $D$ - and  $I$ -optimality problems and leading to the designs of Fig. 3, but extended to  $D$ - and  $I$ -robustness. We again discretize the design space and as an example let  $\mathbf{f}(x)$  contain the quadratic spline wavelets of order  $r = 3$ . The solutions turn out to depend on  $\tau$  and  $\sigma$  only through their ratio, which in this case we take to be 1. Then the  $I$ -robust design is pictured in Fig. 4(a); compare with the  $I$ -optimal design in Fig. 1.

A common feature, illustrated here, is that the robust designs can roughly be described as optimal designs in which replicates are replaced by clusters of nearby but distinct points. The exact implementation of the  $I$ -robust design, with  $n = 50$  and applied to the same data as used in Fig. 3, is in Fig. 4(b). Compare with the  $I$ -optimal design for  $r = 3$  from Fig. 3 ( $\mathcal{D}_{\xi} = 2.968$ ,  $\mathcal{I}_{\xi} = 810.3$ ,  $\|\hat{m} - m\| = 16.65$ ). Again we see very common features of robust solutions—the  $I$ -robust design results in smaller biases, as measured by  $\|\hat{m} - m\|$ , in the face of model misspecification, at the cost of somewhat larger measures of variation when the fitted model is exactly correct.

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## Appendix

**Proof of Lemma 1.** (i) Let  $v \in V_0[0, 1]$ , so that  $v(x) = v_0(x)I_{[0,1]}(x)$  for a function  $v_0 \in V_0$ . Then  $v_0$  may be written as  $v_0(x) = \sum_{k \in \mathcal{K}_0} \alpha_k \gamma(x - k)$ . Since  $k \notin \mathcal{K}_0 \Rightarrow \gamma(x - k) = 0$  a.e.  $x \in [0, 1]$ , we have  $v(x) = \sum_{k \in \mathcal{K}_0} \alpha_k \gamma(x - k)I_{[0,1]}(x)$ . Thus the independent set  $\{\gamma(x - k)I_{[0,1]}(x) \mid k \in \mathcal{K}_0\}$  spans  $V_0[0, 1]$ .

(ii) Let  $v \in V_r[0, 1]$ , and write  $v(x) = \sum_{i=0}^{2^r-1} I_{[\frac{i}{2^r}, \frac{i+1}{2^r}]}(x)v_r(x)$  for some  $v_r \in V_r$ . Then since  $v_r(2^{-r}x) \in V_0$  we have

$$v(2^{-r}x) = \sum_{i=0}^{2^r-1} I_{[i, i+1]}(x) \sum_{j \in \mathcal{Z}} \alpha_j \gamma(x - j) = \sum_{i=0}^{2^r-1} f_i(x - i),$$

where  $f_i(t) = \sum_{j \in \mathcal{Z}} \alpha_{i+j} \gamma(t - j)I_{[0,1]}(t) \in V_0[0, 1]$ . By (i) of this lemma we have  $f_i(t) = \sum_{j \in \mathcal{K}_0} \alpha_{i+j} \gamma(t - j)I_{[0,1]}(t)$  and so

$$\begin{aligned} v(x) &= \sum_{i=0}^{2^r-1} \sum_{j \in \mathcal{K}_0} \alpha_{i+j} \gamma(2^r x - (i + j)) I_{[\frac{i}{2^r}, \frac{i+1}{2^r}]}(x) \\ &= \sum_{k \in \mathcal{K}_r} \alpha_k \gamma(2^r x - k) \sum_{i=0}^{2^r-1} I_{[\frac{i}{2^r}, \frac{i+1}{2^r}]}(x) \\ &= \sum_{k \in \mathcal{K}_r} \alpha_k \gamma(2^r x - k). \end{aligned}$$

Thus the set  $\{\gamma(2^r x - k)I_{[0,1]}(x) \mid k \in \mathcal{K}_r\}$  spans  $V_r[0, 1]$ . To see that the elements are linearly independent, suppose that

$$\sum_{k \in \mathcal{K}_r} \alpha_k \gamma(2^r x - k) \equiv 0 \quad \text{for } x \in [0, 1]. \quad (\text{A.1})$$

For fixed  $i = 0, \dots, 2^r - 1$  let  $x \in [\frac{i}{2^r}, \frac{i+1}{2^r}]$  and put  $y = 2^r x - i \in [0, 1]$ . Then with  $j = k - i$ , (A.1) gives  $\sum_{j \in \mathcal{K}_r - i} \alpha_{j+i} \gamma(y - j) \equiv 0$  for  $y \in [0, 1]$ . Since  $\mathcal{K}_r - i = \{k - i \mid k \in \mathcal{K}_r\} \subset \mathcal{K}_0$ , the above identity implies that  $\alpha_{j+i} = 0$  for  $j \in \mathcal{K}_r - i$ . Since  $i$  is arbitrary,  $\alpha_k = 0$  for all  $k \in \mathcal{K}_r$ .

(iii) The set  $\{\phi_{r,k}(x)I_{[0,1]}(x) \mid k \in \mathcal{Z}\}$  spans  $V_r[0, 1]$  and hence contains a basis, necessarily of the same cardinality as  $\mathcal{K}_r$ . ■

**Elfving's theorem.** Let  $V_+ = \{\mathbf{f}(x) : x \in [0, 1]\}$ ,  $V_- = \{-\mathbf{f}(x) : x \in [0, 1]\}$  and  $V = \text{conv}\{V_+ \cup V_-\}$ . A design  $\xi$  is  $c$ -optimal if and only if there exists a measurable function  $\eta(x)$  satisfying  $|\eta(x)| \equiv 1$  such that (1)  $\int_0^1 \eta(x) \mathbf{f}(x) d\xi = \beta \mathbf{c}$  for some constant  $\beta$ ; (2)  $\beta \mathbf{c}$  is a boundary point of  $V$ . Moreover  $\beta \mathbf{c}$  lies on the boundary of  $V$  if and only if  $\beta^{-2} = \min_{\xi} \{\mathbf{c}^T \mathbf{M}^+(\xi) \mathbf{c}\}$ .

**Lemma 2** (Of Studden, 1968). A vector  $\mathbf{c} \in V$ , which can be put in the form  $\mathbf{c} = \sum_{i=1}^n w_i h_i \mathbf{f}(x_i)$ , with  $|w_i| = 1$ ,  $h_i > 0$  and  $\sum_{i=1}^n h_i = 1$ , lies on the boundary of  $V$  if and only if there exists a nontrivial linear form  $u(x) = \sum_{k=0}^{2^r} a_k f_k(x)$  such that  $|u(x)| \leq 1$  for  $x \in [0, 1]$ ,  $w_i u(x_i) = 1$ ,  $i = 1, 2, \dots, n$ , and  $\sum_{k=0}^{2^r} a_k c_k = 1$ .

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